100 — DERIVE PROTEIN SEQUENCE INFORMATION

102 — ASSIGN PROTEIN SUPERFAMILY OR IDENTIFY RELATED PROTEINS

104 — ASSEMBLE PROTEIN STRUCTURE FROM TEMPLATES

106A — AB INITIO LOOP PREDICTIONS

106B — AB INITIO SECONDARY STRUCTURE GENERATION

110 — ENERGETICALLY REFINE STRUCTURE

FIX PROBLEMS

112 — EVALUATE QUALITY OF STRUCTURE

118

114 — IS MODEL SATISFACTORY?

NO

116

120 — YES

122A — CALCULATE STRUCTURAL AND/OR PHYSICAL PROPERTIES

122B — OBTAIN ASSOCIATED CLINICAL DATA

124 — INPUT INTO STRUCTURAL POLYMORPHISM DATABASE

FIG. I

200 — ACQUIRE PATIENT DATA FOR A GENE EXHIBITING GENETIC POLYMORPHISMS

202 — DERIVE PROTEIN SEQUENCE INFORMATION

204 — HAS THE 3-D STRUCTURE OF THE NATIVE PROTEIN BEEN DETERMINED?

206 — YES

210 — NO   212

208
PERFORM MULTIPLE SEQUENCE ANALYSIS TO
DETERMINE EXACT AMINO ACID VARIATIONS

DETERMINE STRUCTURE BY
PHYSIOCHEMICAL METHODS

214 — GENERATE 3-D STRUCTURAL MODELS FOR ALL VARIANTS

216 — ENERGETICALLY REFINE MODEL STRUCTURES

218 — EVALUATE THE QUALITY OF ALL MODELS

FIX PROBLEMS

224

220 — ARE THE MODELS SATISFACTORY?

226 — YES

222 — NO

228
APPLY STRUCTURE-BASED DRUG DESIGN METHODS TO IDENTIFY
POTENTIAL NEW DRUGS THAT BIND TO THE STRUCTURAL VARIANT MODELS

FIG. 2

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Sheet 3 of 46
Title: Use of Computationally Derived Protein Structures of Genetic Polymorphisms in
Pharmacogenomics for Drug Design and Clinical Applications
Serial No. 09/709,905   Applicants: Ramnarayan et al.
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RECEIVED

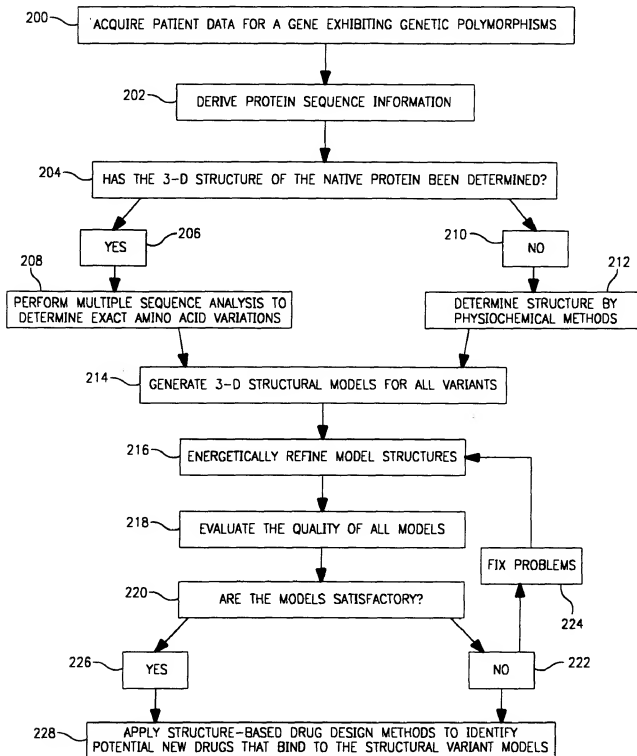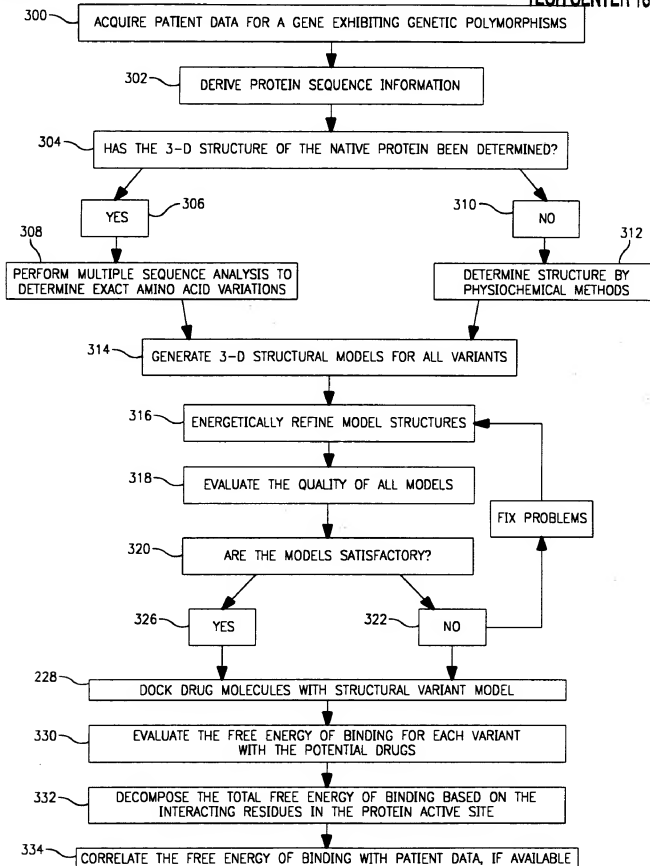OCT 2 4 2002

TECH CENTER 1600/2900

300 — ACQUIRE PATIENT DATA FOR A GENE EXHIBITING GENETIC POLYMORPHISMS

302 — DERIVE PROTEIN SEQUENCE INFORMATION

304 — HAS THE 3-D STRUCTURE OF THE NATIVE PROTEIN BEEN DETERMINED?

306 — YES

310 — NO

308 — PERFORM MULTIPLE SEQUENCE ANALYSIS TO DETERMINE EXACT AMINO ACID VARIATIONS

312 — DETERMINE STRUCTURE BY PHYSIOCHEMICAL METHODS

314 — GENERATE 3-D STRUCTURAL MODELS FOR ALL VARIANTS

316 — ENERGETICALLY REFINE MODEL STRUCTURES

318 — EVALUATE THE QUALITY OF ALL MODELS

FIX PROBLEMS

320 — ARE THE MODELS SATISFACTORY?

326 — YES

322 — NO

228 — DOCK DRUG MOLECULES WITH STRUCTURAL VARIANT MODEL

330 — EVALUATE THE FREE ENERGY OF BINDING FOR EACH VARIANT WITH THE POTENTIAL DRUGS

332 — DECOMPOSE THE TOTAL FREE ENERGY OF BINDING BASED ON THE INTERACTING RESIDUES IN THE PROTEIN ACTIVE SITE

334 — CORRELATE THE FREE ENERGY OF BINDING WITH PATIENT DATA, IF AVAILABLE

FIG. 3

COMPARISON OF CALCULATED VERUS EXPERIMENTAL BINDING
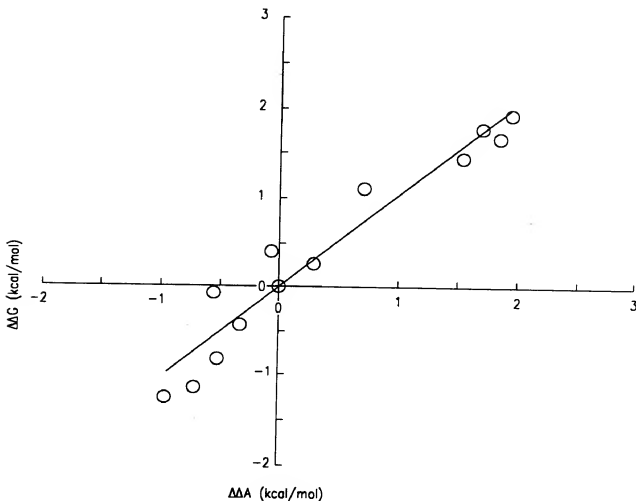FREE ENERGY CHANGES

FIG. 5

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Pharmacogenomics for Drug Design and Clinical Applications
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Date of Filing: 11/10/00   Attorney Docket No. 24737-1906C
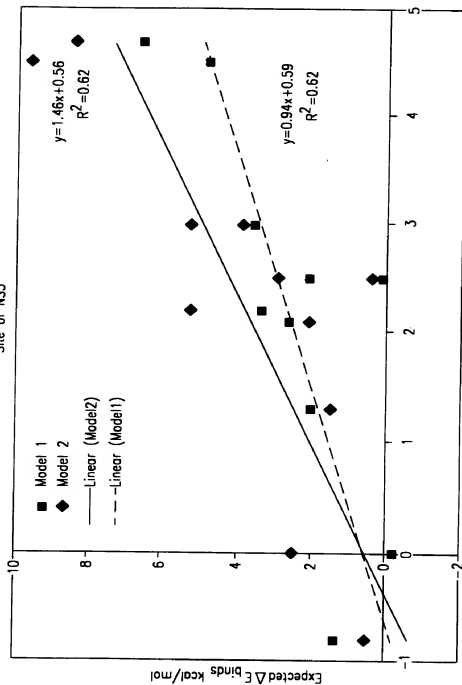
FIG. 4

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Sheet 6 of 46
Title: Use of Computationally Derived Protein Structures of Genetic Polymorphisms in
Pharmacogenomics for Drug Design and Clinical Applications
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HIV PROTEASE INHIBITORS APPROVED BY FDA

SAQUINAVIR

NELFINAVIR

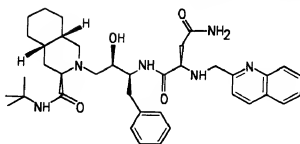INDINAVIR

AMPRENAVIR

RITONAVIR

FIG. 6

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Title: Use of Computationally Derived Protein Structures of Genetic Polymorphisms in
Pharmacogenomics for Drug Design and Clinical Applications
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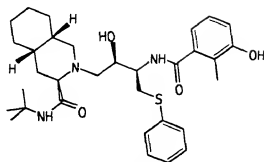Date of Filing: 11/10/00   Attorney Docket No. 24737-1906C

FIG. 7

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Title: Use of Computationally Derived Protein Structures of Genetic Polymorphisms in
Pharmacogenomics for Drug Design and Clinical Applications
Serial No. 09/709,905   Applicants: Ramnarayan et al.
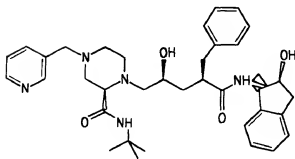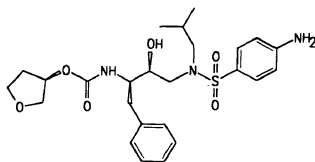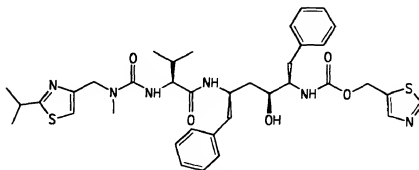Date of Filing: 11/10/00   Attorney Docket No. 24737-1906C
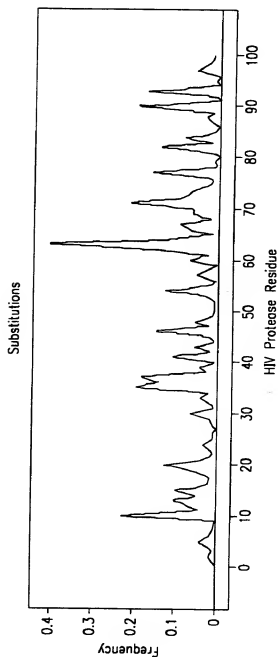
ATOM	1	N	PRO A	1	-3.433	7.956	34.152
ATOM	2	CA	PRO A	1	-2.653	6.918	34.784
ATOM	3	C	PRO A	1	-1.242	7.005	34.259
ATOM	4	O	PRO A	1	-0.950	7.638	33.216
ATOM	5	CB	PRO A	1	-3.281	5.601	34.262
ATOM	6	CG	PRO A	1	-4.191	5.995	33.118
ATOM	7	CD	PRO A	1	-4.547	7.461	33.339
ATOM	8	1H	PRO A	1	-2.845	8.493	33.547
ATOM	9	2H	PRO A	1	-3.824	8.552	34.853
ATOM	10	N	GLN A	2	-0.259	6.464	35.001
ATOM	11	H	GLN A	2	-0.475	6.057	35.889
ATOM	12	CA	GLN A	2	1.115	6.443	34.568
ATOM	13	C	GLN A	2	1.452	4.993	34.301
ATOM	14	O	GLN A	2	1.379	4.106	35.173
ATOM	15	CB	GLN A	2	2.070	6.966	35.653
ATOM	16	CG	GLN A	2	3.549	6.859	35.240
ATOM	17	CD	GLN A	2	4.490	7.744	36.054
ATOM	18	OE1	GLN A	2	4.771	8.888	35.719
ATOM	19	NE2	GLN A	2	4.980	7.190	37.144
ATOM	20	1HE2	GLN A	2	5.605	7.702	37.734
ATOM	21	2HE2	GLN A	2	4.731	6.253	37.390
ATOM	22	N	ILE A	3	1.784	4.644	33.037
ATOM	23	H	ILE A	3	1.876	5.351	32.336
ATOM	24	CA	ILE A	3	2.013	3.257	32.665
ATOM	25	C	ILE A	3	3.505	3.028	32.473
ATOM	26	O	ILE A	3	4.242	3.777	31.787
ATOM	27	CB	ILE A	3	1.226	2.944	31.370
ATOM	28	CG1	ILE A	3	-0.274	3.239	31.603
ATOM	29	CG2	ILE A	3	1.427	1.480	30.901
ATOM	30	CD1	ILE A	3	-1.089	3.219	30.322
ATOM	31	N	THR A	4	4.071	2.032	33.177
ATOM	32	H	THR A	4	3.525	1.525	33.844
ATOM	33	CA	THR A	4	5.451	1.661	33.007
ATOM	34	C	THR A	4	5.515	0.637	31.901
ATOM	35	O	THR A	4	4.490	0.143	31.397
ATOM	36	CB	THR A	4	6.051	1.125	34.324
ATOM	37	OG1	THR A	4	5.224	0.069	34.791
ATOM	38	HG1	THR A	4	5.589	-0.299	35.646
ATOM	39	CG2	THR A	4	6.085	2.212	35.431
ATOM	40	N	LEU A	5	6.677	0.281	31.405
ATOM	41	H	LEU A	5	7.518	0.530	31.885
ATOM	42	CA	LEU A	5	6.754	-0.464	30.177
ATOM	43	C	LEU A	5	7.432	-1.813	30.356
ATOM	44	O	LEU A	5	7.940	-2.464	29.426
ATOM	45	CB	LEU A	5	7.459	0.394	29.128
ATOM	46	CG	LEU A	5	6.668	1.671	28.775
ATOM	47	CD1	LEU A	5	7.493	2.649	27.939
ATOM	48	CD2	LEU A	5	5.345	1.307	28.099
ATOM	49	N	TRP A	6	7.420	-2.351	31.594
ATOM	50	H	TRP A	6	7.030	-1.833	32.356
ATOM	51	CA	TRP A	6	7.958	-3.669	31.865
ATOM	52	C	TRP A	6	7.071	-4.697	31.204
ATOM	53	O	TRP A	6	7.520	-5.798	30.828
ATOM	54	CB	TRP A	6	8.099	-3.913	33.367
ATOM	55	CG	TRP A	6	9.041	-2.974	34.070

FIG. 11A

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Pharmacogenomics for Drug Design and Clinical Applications
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ATOM	56	CD1	TRP	A	6	8.745	-1.769	34.646
ATOM	57	CD2	TRP	A	6	10.449	-3.171	34.273
ATOM	58	NE1	TRP	A	6	9.875	-1.209	35.190
ATOM	59	HE1	TRP	A	6	9.930	-0.332	35.668
ATOM	60	CE2	TRP	A	6	10.932	-2.048	34.974
ATOM	61	CE3	TRP	A	6	11.334	-4.190	33.924
ATOM	62	CZ2	TRP	A	6	12.257	-1.917	35.333
ATOM	63	CZ3	TRP	A	6	12.650	-4.065	34.278
ATOM	64	CH2	TRP	A	6	13.106	-2.942	34.974
ATOM	65	N	GLN	A	7	5.773	-4.448	30.973
ATOM	66	H	GLN	A	7	5.354	-3.619	31.343
ATOM	67	CA	GLN	A	7	4.952	-5.339	30.205
ATOM	68	C	GLN	A	7	4.438	-4.569	29.033
ATOM	69	O	GLN	A	7	4.433	-3.321	29.000
ATOM	70	CB	GLN	A	7	3.712	-5.693	30.969
ATOM	71	CG	GLN	A	7	4.015	-6.467	32.210
ATOM	72	CD	GLN	A	7	2.734	-6.678	32.917
ATOM	73	OE1	GLN	A	7	2.053	-7.681	32.712
ATOM	74	NE2	GLN	A	7	2.356	-5.682	33.736
ATOM	75	1HE2	GLN	A	7	1.501	-5.748	34.251
ATOM	76	2HE2	GLN	A	7	2.926	-4.867	33.837
ATOM	77	N	ARG	A	8	3.777	-5.239	28.078
ATOM	78	H	ARG	A	8	3.688	-6.233	28.142
ATOM	79	CA	ARG	A	8	3.183	-4.568	26.948
ATOM	80	C	ARG	A	8	2.117	-3.648	27.461
ATOM	81	O	ARG	A	8	1.333	-3.965	28.387
ATOM	82	CB	ARG	A	8	2.574	-5.555	25.975
ATOM	83	CG	ARG	A	8	3.532	-6.593	25.437
ATOM	84	CD	ARG	A	8	2.842	-7.610	24.579
ATOM	85	NE	ARG	A	8	3.787	-8.487	23.900
ATOM	86	HE	ARG	A	8	4.762	-8.279	23.982
ATOM	87	CZ	ARG	A	8	3.405	-9.541	23.185
ATOM	88	NH1	ARG	A	8	2.125	-9.871	23.052
ATOM	89	2HH1	ARG	A	8	1.418	-9.321	23.496
ATOM	90	1HH1	ARG	A	8	1.869	-10.670	22.508
ATOM	91	NH2	ARG	A	8	4.332	-10.286	22.589
ATOM	92	1HH2	ARG	A	8	4.062	-11.082	22.048
ATOM	93	2HH2	ARG	A	8	5.299	-10.050	22.682
ATOM	94	N	PRO	A	9	1.990	-2.428	26.938
ATOM	95	CA	PRO	A	9	1.001	-1.462	27.440
ATOM	96	C	PRO	A	9	-0.365	-1.697	26.821
ATOM	97	O	PRO	A	9	-0.918	-0.935	26.008
ATOM	98	CB	PRO	A	9	1.572	-0.112	27.041
ATOM	99	CG	PRO	A	9	2.553	-0.404	25.931
ATOM	100	CD	PRO	A	9	3.024	-1.820	26.084
ATOM	101	N	LEU	A	10	-1.028	-2.803	27.227
ATOM	102	H	LEU	A	10	-0.616	-3.404	27.912
ATOM	103	CA	LEU	A	10	-2.319	-3.143	26.698
ATOM	104	C	LEU	A	10	-3.390	-2.565	27.591
ATOM	105	O	LEU	A	10	-3.336	-2.632	28.831
ATOM	106	CB	LEU	A	10	-2.451	-4.651	26.709
ATOM	107	CG	LEU	A	10	-1.483	-5.316	25.756
ATOM	108	CD1	LEU	A	10	-1.159	-6.740	26.212
ATOM	109	CD2	LEU	A	10	-2.083	-5.262	24.322
ATOM	110	N	VAL	A	11	-4.447	-1.952	27.033
ATOM	111	H	VAL	A	11	-4.507	-1.875	26.038

FIG. I IB

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Title: Use of Computationally Derived Protein Structures of Genetic Polymorphisms in
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ATOM	112	CA	VAL A	11	-5.506	-1.398	27.835
ATOM	113	C	VAL A	11	-6.827	-1.857	27.268
ATOM	114	O	VAL A	11	-6.924	-2.490	26.198
ATOM	115	CB	VAL A	11	-5.420	0.143	27.897
ATOM	116	CG1	VAL A	11	-4.117	0.595	28.551
ATOM	117	CG2	VAL A	11	-5.549	0.787	26.497
ATOM	118	N	THR A	12	-7.954	-1.592	27.978
ATOM	119	H	THR A	12	-7.884	-1.141	28.868
ATOM	120	CA	THR A	12	-9.301	-1.942	27.496
ATOM	121	C	THR A	12	-9.889	-0.726	26.795
ATOM	122	O	THR A	12	-9.856	0.436	27.247
ATOM	123	CB	THR A	12	-10.225	-2.385	28.659
ATOM	124	OG1	THR A	12	-9.596	-3.458	29.338
ATOM	125	HG1	THR A	12	-10.170	-3.766	30.096
ATOM	126	CG2	THR A	12	-11.579	-2.895	28.156
ATOM	127	N	ILE A	13	-10.449	-0.932	25.594
ATOM	128	H	ILE A	13	-10.409	-1.841	25.178
ATOM	129	CA	ILE A	13	-11.112	0.133	24.882
ATOM	130	C	ILE A	13	-12.553	-0.292	24.693
ATOM	131	O	ILE A	13	-12.935	-1.469	24.821
ATOM	132	CB	ILE A	13	-10.432	0.364	23.511
ATOM	133	CG1	ILE A	13	-10.466	-0.896	22.628
ATOM	134	CG2	ILE A	13	-8.986	0.806	23.747
ATOM	135	CD1	ILE A	13	-9.755	-0.745	21.294
ATOM	136	N	LYS A	14	-13.470	0.658	24.438
ATOM	137	H	LYS A	14	-13.209	1.622	24.481
ATOM	138	CA	LYS A	14	-14.838	0.330	24.100
ATOM	139	C	LYS A	14	-15.088	0.877	22.719
ATOM	140	O	LYS A	14	-14.859	2.059	22.375
ATOM	141	CB	LYS A	14	-15.855	0.916	25.099
ATOM	142	CG	LYS A	14	-17.325	0.518	24.864
ATOM	143	CD	LYS A	14	-18.078	0.146	26.166
ATOM	144	CE	LYS A	14	-18.826	1.342	26.810
ATOM	145	NZ	LYS A	14	-19.316	0.929	28.173
ATOM	146	1HZ	LYS A	14	-19.801	1.693	28.599
ATOM	147	3HZ	LYS A	14	-18.536	0.670	28.743
ATOM	148	2HZ	LYS A	14	-19.936	0.150	28.082
ATOM	149	N	ILE A	15	-15.535	0.005	21.798
ATOM	150	H	ILE A	15	-15.806	-0.916	22.078
ATOM	151	CA	ILE A	15	-15.642	0.347	20.400
ATOM	152	C	ILE A	15	-16.894	-0.328	19.887
ATOM	153	O	ILE A	15	-17.115	-1.542	20.041
ATOM	154	CB	ILE A	15	-14.382	-0.132	19.639
ATOM	155	CG1	ILE A	15	-14.478	0.148	18.125
ATOM	156	CG2	ILE A	15	-14.082	-1.623	19.880
ATOM	157	CD1	ILE A	15	-14.237	1.603	17.796
ATOM	158	N	GLY A	16	-17.843	0.435	19.308
ATOM	159	H	GLY A	16	-17.720	1.426	19.260
ATOM	160	CA	GLY A	16	-19.053	-0.143	18.745
ATOM	161	C	GLY A	16	-19.897	-0.817	19.789
ATOM	162	O	GLY A	16	-20.774	-1.668	19.516
ATOM	163	N	GLY A	17	-19.712	-0.493	21.088
ATOM	164	H	GLY A	17	-19.038	0.204	21.334
ATOM	165	CA	GLY A	17	-20.464	-1.126	22.160
ATOM	166	C	GLY A	17	-19.718	-2.335	22.653
ATOM	167	O	GLY A	17	-20.147	-3.098	23.540

FIG. I IC

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Title: Use of Computationally Derived Protein Structures of Genetic Polymorphisms in
Pharmacogenomics for Drug Design and Clinical Applications
Serial No. 09/709,905   Applicants: Ramnarayan et al.
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ATOM	168	N	GLN A	18	-18.507	-2.591	22.121
ATOM	169	H	GLN A	18	-18.059	-1.900	21.554
ATOM	170	CA	GLN A	18	-17.806	-3.830	22.326
ATOM	171	C	GLN A	18	-16.552	-3.549	23.123
ATOM	172	O	GLN A	18	-15.887	-2.508	22.945
ATOM	173	CB	GLN A	18	-17.393	-4.294	20.928
ATOM	174	CG	GLN A	18	-16.911	-5.734	20.788
ATOM	175	CD	GLN A	18	-18.018	-6.728	20.613
ATOM	176	OE1	GLN A	18	-19.131	-6.574	21.152
ATOM	177	NE2	GLN A	18	-17.722	-7.773	19.857
ATOM	178	1HE2	GLN A	18	-18.404	-8.484	19.689
ATOM	179	2HE2	GLN A	18	-16.814	-7.860	19.448
ATOM	180	N	LEU A	19	-16.133	-4.397	24.087
ATOM	181	H	LEU A	19	-16.682	-5.202	24.312
ATOM	182	CA	LEU A	19	-14.909	-4.178	24.808
ATOM	183	C	LEU A	19	-13.799	-4.912	24.090
ATOM	184	O	LEU A	19	-13.989	-6.018	23.558
ATOM	185	CB	LEU A	19	-14.982	-4.714	26.254
ATOM	186	CG	LEU A	19	-15.490	-3.778	27.374
ATOM	187	CD1	LEU A	19	-16.392	-2.639	26.856
ATOM	188	CD2	LEU A	19	-16.208	-4.516	28.465
ATOM	189	N	LYS A	20	-12.603	-4.372	23.978
ATOM	190	H	LYS A	20	-12.442	-3.448	24.324
ATOM	191	CA	LYS A	20	-11.507	-5.082	23.365
ATOM	192	C	LYS A	20	-10.266	-4.618	24.062
ATOM	193	O	LYS A	20	-10.228	-3.611	24.816
ATOM	194	CB	LYS A	20	-11.397	-4.798	21.875
ATOM	195	CG	LYS A	20	-12.558	-5.356	21.100
ATOM	196	CD	LYS A	20	-12.537	-4.988	19.615
ATOM	197	CE	LYS A	20	-13.414	-5.958	18.827
ATOM	198	NZ	LYS A	20	-12.681	-7.208	18.639
ATOM	199	1HZ	LYS A	20	-13.247	-7.852	18.123
ATOM	200	3HZ	LYS A	20	-12.458	-7.601	19.531
ATOM	201	2HZ	LYS A	20	-11.837	-7.027	18.134
ATOM	202	N	GLU A	21	-9.150	-5.357	23.893
ATOM	203	H	GLU A	21	-9.185	-6.188	23.338
ATOM	204	CA	GLU A	21	-7.890	-4.997	24.486
ATOM	205	C	GLU A	21	-7.001	-4.462	23.390
ATOM	206	O	GLU A	21	-6.970	-4.992	22.258
ATOM	207	CB	GLU A	21	-7.268	-6.260	25.051
ATOM	208	CG	GLU A	21	-5.835	-6.140	25.480
ATOM	209	CD	GLU A	21	-5.405	-7.352	26.275
ATOM	210	OE1	GLU A	21	-5.624	-7.343	27.508
ATOM	211	OE2	GLU A	21	-4.852	-8.309	25.684
ATOM	212	N	ALA A	22	-6.239	-3.369	23.595
ATOM	213	H	ALA A	22	-6.223	-2.938	24.497
ATOM	214	CA	ALA A	22	-5.419	-2.781	22.520
ATOM	215	C	ALA A	22	-4.138	-2.255	23.114
ATOM	216	O	ALA A	22	-3.985	-1.914	24.314
ATOM	217	CB	ALA A	22	-6.134	-1.657	21.821
ATOM	218	N	LEU A	23	-3.121	-2.091	22.240
ATOM	219	H	LEU A	23	-3.279	-2.236	21.263
ATOM	220	CA	LEU A	23	-1.797	-1.712	22.640
ATOM	221	C	LEU A	23	-1.660	-0.230	22.443
ATOM	222	O	LEU A	23	-2.020	0.349	21.402
ATOM	223	CB	LEU A	23	-0.814	-2.486	21.732

FIG. 1 ID

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ATOM	224	CG	LEU A	23	0.705	-2.448	21.991
ATOM	225	CD1	LEU A	23	1.088	-3.400	23.124
ATOM	226	CD2	LEU A	23	1.462	-2.878	20.708
ATOM	227	N	LEU A	24	-1.192	0.530	23.463
ATOM	228	H	LEU A	24	-1.015	0.110	24.353
ATOM	229	CA	LEU A	24	-0.935	1.952	23.305
ATOM	230	C	LEU A	24	0.403	2.089	22.609
ATOM	231	O	LEU A	24	1.471	1.717	23.130
ATOM	232	CB	LEU A	24	-0.921	2.609	24.681
ATOM	233	CG	LEU A	24	-2.220	2.492	25.477
ATOM	234	CD1	LEU A	24	-2.063	3.291	26.772
ATOM	235	CD2	LEU A	24	-3.419	3.000	24.691
ATOM	236	N	ASP A	25	0.454	2.590	21.397
ATOM	237	H	ASP A	25	-0.334	3.085	21.032
ATOM	238	CA	ASP A	25	1.642	2.423	20.605
ATOM	239	C	ASP A	25	2.130	3.750	20.059
ATOM	240	O	ASP A	25	1.568	4.320	19.110
ATOM	241	CB	ASP A	25	1.263	1.435	19.486
ATOM	242	CG	ASP A	25	2.428	1.051	18.561
ATOM	243	OD1	ASP A	25	3.546	1.540	18.729
ATOM	244	OD2	ASP A	25	2.164	0.241	17.658
ATOM	245	N	THR A	26	3.203	4.337	20.605
ATOM	246	H	THR A	26	3.694	3.880	21.346
ATOM	247	CA	THR A	26	3.691	5.652	20.144
ATOM	248	C	THR A	26	4.397	5.583	18.778
ATOM	249	O	THR A	26	4.642	6.587	18.079
ATOM	250	CB	THR A	26	4.596	6.219	21.217
ATOM	251	OG1	THR A	26	5.716	5.324	21.386
ATOM	252	HG1	THR A	26	6.332	5.676	22.091
ATOM	253	CG2	THR A	26	3.878	6.320	22.577
ATOM	254	N	GLY A	27	4.757	4.377	18.298
ATOM	255	H	GLY A	27	4.526	3.550	18.811
ATOM	256	CA	GLY A	27	5.481	4.233	17.040
ATOM	257	C	GLY A	27	4.520	4.190	15.886
ATOM	258	O	GLY A	27	4.908	4.242	14.696
ATOM	259	N	ALA A	28	3.197	4.084	16.117
ATOM	260	H	ALA A	28	2.856	4.091	17.057
ATOM	261	CA	ALA A	28	2.213	3.955	15.018
ATOM	262	C	ALA A	28	1.598	5.299	14.750
ATOM	263	O	ALA A	28	1.062	5.982	15.650
ATOM	264	CB	ALA A	28	1.117	2.980	15.390
ATOM	265	N	ASP A	29	1.503	5.744	13.490
ATOM	266	H	ASP A	29	1.912	5.216	12.746
ATOM	267	CA	ASP A	29	0.810	6.984	13.213
ATOM	268	C	ASP A	29	-0.666	6.724	13.327
ATOM	269	O	ASP A	29	-1.488	7.637	13.568
ATOM	270	CB	ASP A	29	1.009	7.433	11.775
ATOM	271	CG	ASP A	29	2.439	7.882	11.412
ATOM	272	OD1	ASP A	29	3.360	7.856	12.269
ATOM	273	OD2	ASP A	29	2.606	8.253	10.252
ATOM	274	N	ASP A	30	-1.143	5.517	12.990
ATOM	275	H	ASP A	30	-0.508	4.769	12.800
ATOM	276	CA	ASP A	30	-2.579	5.245	12.887
ATOM	277	C	ASP A	30	-3.057	4.208	13.867
ATOM	278	O	ASP A	30	-2.284	3.483	14.546
ATOM	279	CB	ASP A	30	-2.896	4.758	11.456

FIG. IIE

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ATOM	280	CG	ASP	A	30	-2.495	5.768	10.425
ATOM	281	OD1	ASP	A	30	-3.067	6.871	10.423
ATOM	282	OD2	ASP	A	30	-1.596	5.494	9.618
ATOM	283	N	THR	A	31	-4.393	4.076	14.002
ATOM	284	H	THR	A	31	-5.004	4.700	13.515
ATOM	285	CA	THR	A	31	-5.059	3.062	14.829
ATOM	286	C	THR	A	31	-5.565	1.967	13.913
ATOM	287	O	THR	A	31	-6.223	2.169	12.870
ATOM	288	CB	THR	A	31	-6.212	3.725	15.566
ATOM	289	OG1	THR	A	31	-5.668	4.667	16.474
ATOM	290	HG1	THR	A	31	-6.403	5.122	16.976
ATOM	291	CG2	THR	A	31	-7.044	2.702	16.389
ATOM	292	N	VAL	A	32	-5.187	0.713	14.235
ATOM	293	H	VAL	A	32	-4.649	0.555	15.063
ATOM	294	CA	VAL	A	32	-5.517	-0.462	13.437
ATOM	295	C	VAL	A	32	-6.092	-1.506	14.365
ATOM	296	O	VAL	A	32	-5.502	-1.957	15.365
ATOM	297	CB	VAL	A	32	-4.260	-1.064	12.757
ATOM	298	CG1	VAL	A	32	-4.667	-2.136	11.735
ATOM	299	CG2	VAL	A	32	-3.422	0.017	12.032
ATOM	300	N	LEU	A	33	-7.352	-1.923	14.119
ATOM	301	H	LEU	A	33	-7.867	-1.523	13.361
ATOM	302	CA	LEU	A	33	-7.982	-2.940	14.929
ATOM	303	C	LEU	A	33	-8.174	-4.203	14.107
ATOM	304	O	LEU	A	33	-8.268	-4.247	12.853
ATOM	305	CB	LEU	A	33	-9.336	-2.477	15.408
ATOM	306	CG	LEU	A	33	-9.292	-1.149	16.127
ATOM	307	CD1	LEU	A	33	-10.710	-0.747	16.485
ATOM	308	CD2	LEU	A	33	-8.348	-1.139	17.347
ATOM	309	N	GLU	A	34	-8.296	-5.319	14.782
ATOM	310	H	GLU	A	34	-8.244	-5.302	15.780
ATOM	311	CA	GLU	A	34	-8.503	-6.551	14.086
ATOM	312	C	GLU	A	34	-9.909	-6.549	13.510
ATOM	313	O	GLU	A	34	-10.808	-5.717	13.795
ATOM	314	CB	GLU	A	34	-8.265	-7.750	15.010
ATOM	315	CG	GLU	A	34	-9.259	-7.791	16.165
ATOM	316	CD	GLU	A	34	-8.763	-8.552	17.404
ATOM	317	OE1	GLU	A	34	-7.670	-9.193	17.368
ATOM	318	OE2	GLU	A	34	-9.482	-8.497	18.407
ATOM	319	N	GLU	A	35	-10.152	-7.480	12.568
ATOM	320	H	GLU	A	35	-9.485	-8.208	12.407
ATOM	321	CA	GLU	A	35	-11.352	-7.466	11.773
ATOM	322	C	GLU	A	35	-12.631	-7.520	12.571
ATOM	323	O	GLU	A	35	-12.814	-8.294	13.528
ATOM	324	CB	GLU	A	35	-11.237	-8.536	10.707
ATOM	325	CG	GLU	A	35	-9.945	-8.280	9.907
ATOM	326	CD	GLU	A	35	-9.872	-8.872	8.486
ATOM	327	OE1	GLU	A	35	-10.612	-8.401	7.603
ATOM	328	OE2	GLU	A	35	-9.024	-9.776	8.261
ATOM	329	N	MET	A	36	-13.580	-6.598	12.278
ATOM	330	H	MET	A	36	-13.439	-5.967	11.515
ATOM	331	CA	MET	A	36	-14.819	-6.495	13.052
ATOM	332	C	MET	A	36	-15.826	-5.635	12.271
ATOM	333	O	MET	A	36	-15.514	-4.828	11.371
ATOM	334	CB	MET	A	36	-14.593	-5.845	14.428
ATOM	335	CG	MET	A	36	-14.279	-4.353	14.417

FIG. 1 IF

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ATOM	336	SD	MET	A	36	-14.251	-3.718	16.099
ATOM	337	CE	MET	A	36	-12.487	-3.846	16.409
ATOM	338	N	SER	A	37	-17.130	-5.776	12.590
ATOM	339	H	SER	A	37	-17.399	-6.431	13.296
ATOM	340	CA	SER	A	37	-18.155	-5.005	11.940
ATOM	341	C	SER	A	37	-18.286	-3.693	12.657
ATOM	342	O	SER	A	37	-18.593	-3.624	13.865
ATOM	343	CB	SER	A	37	-19.506	-5.688	12.032
ATOM	344	OG	SER	A	37	-19.455	-7.054	11.718
ATOM	345	HG	SER	A	37	-20.367	-7.457	11.791
ATOM	346	N	LEU	A	38	-18.185	-2.569	11.933
ATOM	347	H	LEU	A	38	-17.956	-2.625	10.952
ATOM	348	CA	LEU	A	38	-18.557	-1.247	12.465
ATOM	349	C	LEU	A	38	-19.630	-0.605	11.572
ATOM	350	O	LEU	A	38	-19.706	-0.939	10.391
ATOM	351	CB	LEU	A	38	-17.315	-0.346	12.588
ATOM	352	CG	LEU	A	38	-16.246	-0.818	13.596
ATOM	353	CD1	LEU	A	38	-14.998	0.073	13.489
ATOM	354	CD2	LEU	A	38	-16.756	-0.787	15.046
ATOM	355	N	PRO	A	39	-20.455	0.321	12.108
ATOM	356	CA	PRO	A	39	-21.460	1.053	11.339
ATOM	357	C	PRO	A	39	-20.824	2.176	10.502
ATOM	358	O	PRO	A	39	-19.654	2.519	10.685
ATOM	359	CB	PRO	A	39	-22.430	1.607	12.389
ATOM	360	CG	PRO	A	39	-21.531	1.845	13.600
ATOM	361	CD	PRO	A	39	-20.539	0.686	13.517
ATOM	362	N	GLY	A	40	-21.620	2.749	9.586
ATOM	363	H	GLY	A	40	-22.569	2.417	9.493
ATOM	364	CA	GLY	A	40	-21.203	3.811	8.678
ATOM	365	C	GLY	A	40	-20.836	3.262	7.298
ATOM	366	O	GLY	A	40	-21.405	2.268	6.845
ATOM	367	N	LYS	A	41	-19.895	3.945	6.631
ATOM	368	H	LYS	A	41	-19.496	4.761	7.071
ATOM	369	CA	LYS	A	41	-19.323	3.558	5.343
ATOM	370	C	LYS	A	41	-17.798	3.757	5.371
ATOM	371	O	LYS	A	41	-17.263	4.462	6.229
ATOM	372	CB	LYS	A	41	-20.025	4.352	4.224
ATOM	373	CG	LYS	A	41	-19.703	3.839	2.810
ATOM	374	CD	LYS	A	41	-20.610	4.486	1.757
ATOM	375	CE	LYS	A	41	-20.240	3.964	0.366
ATOM	376	NZ	LYS	A	41	-21.097	4.552	-0.678
ATOM	377	1HZ	LYS	A	41	-20.824	4.189	-1.580
ATOM	378	3HZ	LYS	A	41	-20.993	5.556	-0.673
ATOM	379	2HZ	LYS	A	41	-22.061	4.311	-0.498
ATOM	380	N	TRP	A	42	-17.104	3.091	4.439
ATOM	381	H	TRP	A	42	-17.620	2.548	3.762
ATOM	382	CA	TRP	A	42	-15.654	2.932	4.423
ATOM	383	C	TRP	A	42	-15.105	2.852	2.994
ATOM	384	O	TRP	A	42	-15.845	2.702	2.021
ATOM	385	CB	TRP	A	42	-15.279	1.675	5.236
ATOM	386	CG	TRP	A	42	-16.214	0.514	5.094
ATOM	387	CD1	TRP	A	42	-16.230	-0.402	4.101
ATOM	388	CD2	TRP	A	42	-17.355	0.203	5.942
ATOM	389	NE1	TRP	A	42	-17.297	-1.260	4.281
ATOM	390	HE1	TRP	A	42	-17.504	-2.015	3.644
ATOM	391	CE2	TRP	A	42	-18.045	-0.914	5.389

FIG. 1 IG

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ATOM	392	CE3	TRP	A	42	-17.896	0.792	7.103
ATOM	393	CZ2	TRP	A	42	-19.224	-1.421	5.959
ATOM	394	CZ3	TRP	A	42	-19.077	0.298	7.675
ATOM	395	CH2	TRP	A	42	-19.741	-0.806	7.112
ATOM	396	N	LYS	A	43	-13.771	2.932	2.911
ATOM	397	H	LYS	A	43	-13.260	3.058	3.773
ATOM	398	CA	LYS	A	43	-12.951	2.802	1.713
ATOM	399	C	LYS	A	43	-11.773	1.859	2.012
ATOM	400	O	LYS	A	43	-11.359	1.760	3.166
ATOM	401	CB	LYS	A	43	-12.451	4.193	1.270
ATOM	402	CG	LYS	A	43	-11.724	4.979	2.383
ATOM	403	CD	LYS	A	43	-11.060	6.267	1.873
ATOM	404	CE	LYS	A	43	-9.784	6.001	1.065
ATOM	405	NZ	LYS	A	43	-8.700	5.458	1.903
ATOM	406	1HZ	LYS	A	43	-7.876	5.315	1.338
ATOM	407	3HZ	LYS	A	43	-8.993	4.576	2.300
ATOM	408	2HZ	LYS	A	43	-8.493	6.108	2.647
ATOM	409	N	PRO	A	44	-11.177	1.197	1.004
ATOM	410	CA	PRO	A	44	-9.947	0.435	1.187
ATOM	411	C	PRO	A	44	-8.760	1.392	1.379
ATOM	412	O	PRO	A	44	-8.711	2.434	0.720
ATOM	413	CB	PRO	A	44	-9.808	-0.393	-0.095
ATOM	414	CG	PRO	A	44	-10.501	0.458	-1.159
ATOM	415	CD	PRO	A	44	-11.630	1.132	-0.380
ATOM	416	N	LYS	A	45	-7.790	1.030	2.240
ATOM	417	H	LYS	A	45	-7.912	0.227	2.824
ATOM	418	CA	LYS	A	45	-6.547	1.747	2.314
ATOM	419	C	LYS	A	45	-5.493	0.683	2.507
ATOM	420	O	LYS	A	45	-5.780	-0.470	2.869
ATOM	421	CB	LYS	A	45	-6.594	2.699	3.524
ATOM	422	CG	LYS	A	45	-5.463	3.744	3.609
ATOM	423	CD	LYS	A	45	-5.340	4.289	5.052
ATOM	424	CE	LYS	A	45	-4.262	5.383	5.204
ATOM	425	NZ	LYS	A	45	-2.907	4.911	4.916
ATOM	426	1HZ	LYS	A	45	-2.260	5.664	5.032
ATOM	427	3HZ	LYS	A	45	-2.864	4.577	3.975
ATOM	428	2HZ	LYS	A	45	-2.672	4.169	5.544
ATOM	429	N	MET	A	46	-4.224	0.949	2.193
ATOM	430	H	MET	A	46	-3.998	1.805	1.728
ATOM	431	CA	MET	A	46	-3.157	0.027	2.509
ATOM	432	C	MET	A	46	-2.417	0.701	3.627
ATOM	433	O	MET	A	46	-2.259	1.937	3.634
ATOM	434	CB	MET	A	46	-2.166	-0.088	1.379
ATOM	435	CG	MET	A	46	-2.782	-0.366	0.053
ATOM	436	SD	MET	A	46	-3.076	-2.108	-0.118
ATOM	437	CE	MET	A	46	-1.417	-2.652	-0.186
ATOM	438	N	ILE	A	47	-1.827	-0.016	4.586
ATOM	439	H	ILE	A	47	-2.010	-0.997	4.655
ATOM	440	CA	ILE	A	47	-0.922	0.586	5.539
ATOM	441	C	ILE	A	47	0.233	-0.372	5.654
ATOM	442	O	ILE	A	47	0.135	-1.584	5.356
ATOM	443	CB	ILE	A	47	-1.550	0.836	6.923
ATOM	444	CG1	ILE	A	47	-2.459	-0.301	7.354
ATOM	445	CG2	ILE	A	47	-2.248	2.164	6.995
ATOM	446	CD1	ILE	A	47	-1.724	-1.336	8.111
ATOM	447	N	GLY	A	48	1.420	0.089	6.043

FIG. I IH

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ATOM	448	H	GLY	A	48	1.509	1.040	6.339
ATOM	449	CA	GLY	A	48	2.584	-0.753	6.048
ATOM	450	C	GLY	A	48	3.280	-0.657	7.376
ATOM	451	O	GLY	A	48	3.050	0.190	8.265
ATOM	452	N	GLY	A	49	4.197	-1.617	7.603
ATOM	453	H	GLY	A	49	4.375	-2.308	6.902
ATOM	454	CA	GLY	A	49	4.936	-1.684	8.828
ATOM	455	C	GLY	A	49	6.105	-2.589	8.533
ATOM	456	O	GLY	A	49	6.482	-2.807	7.370
ATOM	457	N	ILE	A	50	6.761	-3.173	9.552
ATOM	458	H	ILE	A	50	6.552	-2.908	10.493
ATOM	459	CA	ILE	A	50	7.772	-4.184	9.344
ATOM	460	C	ILE	A	50	7.148	-5.317	8.566
ATOM	461	O	ILE	A	50	5.981	-5.734	8.772
ATOM	462	CB	ILE	A	50	8.258	-4.686	10.722
ATOM	463	CG1	ILE	A	50	9.257	-3.714	11.382
ATOM	464	CG2	ILE	A	50	8.813	-6.134	10.693
ATOM	465	CD1	ILE	A	50	10.580	-3.498	10.628
ATOM	466	N	GLY	A	51	7.847	-5.891	7.596
ATOM	467	H	GLY	A	51	8.772	-5.569	7.395
ATOM	468	CA	GLY	A	51	7.265	-6.966	6.850
ATOM	469	C	GLY	A	51	6.519	-6.559	5.591
ATOM	470	O	GLY	A	51	6.430	-7.318	4.634
ATOM	471	N	GLY	A	52	5.886	-5.375	5.517
ATOM	472	H	GLY	A	52	5.990	-4.710	6.257
ATOM	473	CA	GLY	A	52	5.108	-5.227	4.320
ATOM	474	C	GLY	A	52	3.832	-4.415	4.516
ATOM	475	O	GLY	A	52	3.654	-3.624	5.467
ATOM	476	N	PHE	A	53	2.886	-4.518	3.559
ATOM	477	H	PHE	A	53	3.013	-5.161	2.804
ATOM	478	CA	PHE	A	53	1.653	-3.720	3.566
ATOM	479	C	PHE	A	53	0.494	-4.651	3.783
ATOM	480	O	PHE	A	53	0.448	-5.816	3.336
ATOM	481	CB	PHE	A	53	1.424	-3.022	2.221
ATOM	482	CG	PHE	A	53	2.363	-1.896	2.008
ATOM	483	CD1	PHE	A	53	3.615	-2.135	1.447
ATOM	484	CD2	PHE	A	53	2.011	-0.608	2.414
ATOM	485	CE1	PHE	A	53	4.514	-1.087	1.275
ATOM	486	CE2	PHE	A	53	2.925	0.446	2.237
ATOM	487	CZ	PHE	A	53	4.172	0.202	1.668
ATOM	488	N	ILE	A	54	-0.554	-4.173	4.439
ATOM	489	H	ILE	A	54	-0.491	-3.285	4.895
ATOM	490	CA	ILE	A	54	-1.789	-4.911	4.509
ATOM	491	C	ILE	A	54	-2.903	-3.995	4.033
ATOM	492	O	ILE	A	54	-2.751	-2.770	3.855
ATOM	493	CB	ILE	A	54	-2.034	-5.535	5.904
ATOM	494	CG1	ILE	A	54	-2.343	-4.481	6.988
ATOM	495	CG2	ILE	A	54	-0.799	-6.318	6.314
ATOM	496	CD1	ILE	A	54	-3.010	-5.089	8.246
ATOM	497	N	LYS	A	55	-4.029	-4.577	3.560
ATOM	498	H	LYS	A	55	-4.084	-5.574	3.501
ATOM	499	CA	LYS	A	55	-5.177	-3.798	3.129
ATOM	500	C	LYS	A	55	-6.115	-3.726	4.300
ATOM	501	O	LYS	A	55	-6.422	-4.707	5.023
ATOM	502	CB	LYS	A	55	-5.928	-4.461	1.938
ATOM	503	CG	LYS	A	55	-6.853	-3.547	1.106

FIG. 1 II

ATOM	504	CD	LYS	A 55	-8.267	-3.332	1.714
ATOM	505	CE	LYS	A 55	-9.303	-4.392	1.301
ATOM	506	NZ	LYS	A 55	-10.521	-4.453	2.192
ATOM	507	1HZ	LYS	A 55	-11.142	-5.162	1.859
ATOM	508	3HZ	LYS	A 55	-10.987	-3.569	2.180
ATOM	509	2HZ	LYS	A 55	-10.240	-4.669	3.127
ATOM	510	N	VAL	A 56	-6.599	-2.509	4.619
ATOM	511	H	VAL	A 56	-6.337	-1.713	4.073
ATOM	512	CA	VAL	A 56	-7.494	-2.311	5.735
ATOM	513	C	VAL	A 56	-8.711	-1.584	5.236
ATOM	514	O	VAL	A 56	-8.767	-1.029	4.114
ATOM	515	CB	VAL	A 56	-6.759	-1.475	6.812
ATOM	516	CG1	VAL	A 56	-5.569	-2.209	7.385
ATOM	517	CG2	VAL	A 56	-6.287	-0.108	6.268
ATOM	518	N	ARG	A 57	-9.784	-1.539	6.005
ATOM	519	H	ARG	A 57	-9.835	-2.117	6.819
ATOM	520	CA	ARG	A 57	-10.855	-0.648	5.638
ATOM	521	C	ARG	A 57	-10.738	0.534	6.554
ATOM	522	O	ARG	A 57	-10.558	0.449	7.789
ATOM	523	CB	ARG	A 57	-12.219	-1.271	5.835
ATOM	524	CG	ARG	A 57	-12.480	-2.452	4.952
ATOM	525	CD	ARG	A 57	-13.834	-3.051	5.195
ATOM	526	NE	ARG	A 57	-14.122	-4.137	4.270
ATOM	527	HE	ARG	A 57	-13.442	-4.347	3.568
ATOM	528	CZ	ARG	A 57	-15.243	-4.851	4.324
ATOM	529	NH1	ARG	A 57	-16.175	-4.624	5.243
ATOM	530	2HH1	ARG	A 57	-16.044	-3.899	5.920
ATOM	531	1HH1	ARG	A 57	-17.008	-5.178	5.258
ATOM	532	NH2	ARG	A 57	-15.433	-5.822	3.434
ATOM	533	1HH2	ARG	A 57	-16.270	-6.368	3.461
ATOM	534	2HH2	ARG	A 57	-14.738	-6.006	2.738
ATOM	535	N	GLN	A 58	-10.881	1.741	6.036
ATOM	536	H	GLN	A 58	-11.030	1.844	5.053
ATOM	537	CA	GLN	A 58	-10.830	2.922	6.839
ATOM	538	C	GLN	A 58	-12.231	3.342	7.205
ATOM	539	O	GLN	A 58	-13.106	3.608	6.359
ATOM	540	CB	GLN	A 58	-10.208	4.038	6.030
ATOM	541	CG	GLN	A 58	-10.055	5.293	6.817
ATOM	542	CD	GLN	A 58	-9.632	6.411	5.927
ATOM	543	OE1	GLN	A 58	-10.379	7.334	5.662
ATOM	544	NE2	GLN	A 58	-8.412	6.303	5.437
ATOM	545	1HE2	GLN	A 58	-8.047	7.009	4.830
ATOM	546	2HE2	GLN	A 58	-7.843	5.514	5.668
ATOM	547	N	TYR	A 59	-12.527	3.516	8.509
ATOM	548	H	TYR	A 59	-11.877	3.219	9.209
ATOM	549	CA	TYR	A 59	-13.769	4.125	8.933
ATOM	550	C	TYR	A 59	-13.411	5.452	9.565
ATOM	551	O	TYR	A 59	-12.416	5.592	10.310
ATOM	552	CB	TYR	A 59	-14.517	3.252	9.957
ATOM	553	CG	TYR	A 59	-14.287	1.770	9.723
ATOM	554	CD1	TYR	A 59	-13.007	1.269	9.457
ATOM	555	CD2	TYR	A 59	-15.346	0.865	9.766
ATOM	556	CE1	TYR	A 59	-12.797	-0.092	9.240
ATOM	557	CE2	TYR	A 59	-15.148	-0.494	9.551
ATOM	558	CZ	TYR	A 59	-13.873	-0.972	9.287
ATOM	559	OH	TYR	A 59	-13.721	-2.311	9.079

FIG. 1 IJ

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ATOM	560	HH	TYR	A	59	-14.606	-2.771	9.154
ATOM	561	N	ASP	A	60	-14.151	6.542	9.300
ATOM	562	H	ASP	A	60	-14.954	6.464	8.709
ATOM	563	CA	ASP	A	60	-13.822	7.836	9.846
ATOM	564	C	ASP	A	60	-14.782	8.226	10.947
ATOM	565	O	ASP	A	60	-15.941	7.765	11.053
ATOM	566	CB	ASP	A	60	-13.861	8.942	8.769
ATOM	567	CG	ASP	A	60	-12.735	8.830	7.725
ATOM	568	OD1	ASP	A	60	-11.545	8.874	8.075
ATOM	569	OD2	ASP	A	60	-13.060	8.702	6.544
ATOM	570	N	GLN	A	61	-14.339	9.154	11.833
ATOM	571	H	GLN	A	61	-13.385	9.451	11.804
ATOM	572	CA	GLN	A	61	-15.151	9.804	12.885
ATOM	573	C	GLN	A	61	-15.839	8.803	13.802
ATOM	574	O	GLN	A	61	-17.008	8.893	14.229
ATOM	575	CB	GLN	A	61	-16.097	10.908	12.338
ATOM	576	CG	GLN	A	61	-16.239	12.133	13.262
ATOM	577	CD	GLN	A	61	-16.910	13.366	12.629
ATOM	578	OE1	GLN	A	61	-16.509	13.854	11.586
ATOM	579	NE2	GLN	A	61	-17.937	13.887	13.292
ATOM	580	1HE2	GLN	A	61	-18.416	14.689	12.934
ATOM	581	2HE2	GLN	A	61	-18.239	13.482	14.155
ATOM	582	N	ILE	A	62	-15.060	7.760	14.175
ATOM	583	H	ILE	A	62	-14.111	7.714	13.862
ATOM	584	CA	ILE	A	62	-15.557	6.705	15.015
ATOM	585	C	ILE	A	62	-15.251	7.057	16.447
ATOM	586	O	ILE	A	62	-14.198	7.613	16.837
ATOM	587	CB	ILE	A	62	-14.829	5.397	14.653
ATOM	588	CG1	ILE	A	62	-15.253	4.966	13.258
ATOM	589	CG2	ILE	A	62	-15.106	4.271	15.675
ATOM	590	CD1	ILE	A	62	-16.779	4.788	13.116
ATOM	591	N	LEU	A	63	-16.242	6.807	17.320
ATOM	592	H	LEU	A	63	-17.089	6.383	17.000
ATOM	593	CA	LEU	A	63	-16.127	7.131	18.719
ATOM	594	C	LEU	A	63	-15.518	5.942	19.425
ATOM	595	O	LEU	A	63	-15.869	4.753	19.269
ATOM	596	CB	LEU	A	63	-17.512	7.428	19.282
ATOM	597	CG	LEU	A	63	-17.660	7.598	20.813
ATOM	598	CD1	LEU	A	63	-16.711	8.632	21.404
ATOM	599	CD2	LEU	A	63	-19.089	7.963	21.201
ATOM	600	N	ILE	A	64	-14.511	6.211	20.219
ATOM	601	H	ILE	A	64	-14.185	7.153	20.305
ATOM	602	CA	ILE	A	64	-13.862	5.178	20.972
ATOM	603	C	ILE	A	64	-13.529	5.744	22.325
ATOM	604	O	ILE	A	64	-13.396	6.959	22.602
ATOM	605	CB	ILE	A	64	-12.618	4.716	20.231
ATOM	606	CG1	ILE	A	64	-11.925	3.573	20.949
ATOM	607	CG2	ILE	A	64	-11.690	5.865	19.950
ATOM	608	CD1	ILE	A	64	-10.905	2.888	20.062
ATOM	609	N	GLU	A	65	-13.396	4.815	23.294
ATOM	610	H	GLU	A	65	-13.443	3.844	23.059
ATOM	611	CA	GLU	A	65	-13.186	5.174	24.670
ATOM	612	C	GLU	A	65	-12.024	4.360	25.165
ATOM	613	O	GLU	A	65	-11.943	3.112	25.056
ATOM	614	CB	GLU	A	65	-14.459	4.823	25.405
ATOM	615	CG	GLU	A	65	-14.739	5.610	26.646

FIG. 1 IK

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ATOM	616	CD	GLU	A	65	-16.131	5.353	27.115
ATOM	617	OE1	GLU	A	65	-17.090	5.785	26.413
ATOM	618	OE2	GLU	A	65	-16.269	4.708	28.163
ATOM	619	N	ILE	A	66	-10.971	5.008	25.610
ATOM	620	H	ILE	A	66	-11.009	6.002	25.717
ATOM	621	CA	ILE	A	66	-9.762	4.317	25.947
ATOM	622	C	ILE	A	66	-9.571	4.586	27.413
ATOM	623	O	ILE	A	66	-9.422	5.732	27.880
ATOM	624	CB	ILE	A	66	-8.600	4.907	25.126
ATOM	625	CG1	ILE	A	66	-8.838	4.669	23.633
ATOM	626	CG2	ILE	A	66	-7.231	4.326	25.554
ATOM	627	CD1	ILE	A	66	-8.951	5.982	22.856
ATOM	628	N	CYS	A	67	-9.776	3.567	28.261
ATOM	629	H	CYS	A	67	-9.989	2.659	27.902
ATOM	630	CA	CYS	A	67	-9.698	3.740	29.687
ATOM	631	C	CYS	A	67	-10.673	4.871	30.088
ATOM	632	O	CYS	A	67	-10.393	5.716	30.958
ATOM	633	CB	CYS	A	67	-8.251	4.003	30.156
ATOM	634	SG	CYS	A	67	-7.170	2.529	30.217
ATOM	635	N	GLY	A	68	-11.877	4.947	29.499
ATOM	636	H	GLY	A	68	-12.125	4.286	28.791
ATOM	637	CA	GLY	A	68	-12.788	5.984	29.903
ATOM	638	C	GLY	A	68	-12.581	7.322	29.241
ATOM	639	O	GLY	A	68	-13.404	8.253	29.376
ATOM	640	N	HIS	A	69	-11.504	7.545	28.471
ATOM	641	H	HIS	A	69	-10.817	6.827	28.360
ATOM	642	CA	HIS	A	69	-11.305	8.800	27.793
ATOM	643	C	HIS	A	69	-11.838	8.679	26.399
ATOM	644	O	HIS	A	69	-11.516	7.742	25.630
ATOM	645	CB	HIS	A	69	-9.831	9.128	27.724
ATOM	646	CG	HIS	A	69	-9.276	9.286	29.081
ATOM	647	ND1	HIS	A	69	-9.317	10.484	29.778
ATOM	648	HD1	HIS	A	69	-9.688	11.347	29.436
ATOM	649	CD2	HIS	A	69	-8.723	8.352	29.912
ATOM	650	CE1	HIS	A	69	-8.783	10.254	30.947
ATOM	651	NE2	HIS	A	69	-8.405	8.990	31.091
ATOM	652	N	LYS	A	70	-12.768	9.561	25.973
ATOM	653	H	LYS	A	70	-13.084	10.284	26.588
ATOM	654	CA	LYS	A	70	-13.325	9.492	24.646
ATOM	655	C	LYS	A	70	-12.346	10.074	23.653
ATOM	656	O	LYS	A	70	-11.587	11.055	23.864
ATOM	657	CB	LYS	A	70	-14.645	10.285	24.536
ATOM	658	CG	LYS	A	70	-15.837	9.703	25.330
ATOM	659	CD	LYS	A	70	-17.105	10.593	25.286
ATOM	660	CE	LYS	A	70	-18.293	10.011	26.092
ATOM	661	NZ	LYS	A	70	-18.802	8.702	25.608
ATOM	662	1HZ	LYS	A	70	-19.563	8.406	26.185
ATOM	663	3HZ	LYS	A	70	-18.069	8.023	25.650
ATOM	664	2HZ	LYS	A	70	-19.116	8.795	24.663
ATOM	665	N	ALA	A	71	-12.323	9.485	22.446
ATOM	666	H	ALA	A	71	-12.813	8.625	22.305
ATOM	667	CA	ALA	A	71	-11.616	10.044	21.333
ATOM	668	C	ALA	A	71	-12.529	9.795	20.171
ATOM	669	O	ALA	A	71	-13.351	8.850	20.146
ATOM	670	CB	ALA	A	71	-10.292	9.358	21.143
ATOM	671	N	ILE	A	72	-12.559	10.685	19.149

FIG. 1IL

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ATOM	672	H	ILE A	72	-12.006	11.517	19.200
ATOM	673	CA	ILE A	72	-13.376	10.474	17.963
ATOM	674	C	ILE A	72	-12.480	10.662	16.771
ATOM	675	O	ILE A	72	-11.858	11.720	16.550
ATOM	676	CB	ILE A	72	-14.541	11.464	17.882
ATOM	677	CG1	ILE A	72	-15.306	11.455	19.196
ATOM	678	CG2	ILE A	72	-15.429	11.203	16.651
ATOM	679	CD1	ILE A	72	-16.446	12.415	19.176
ATOM	680	N	GLY A	73	-12.252	9.633	15.958
ATOM	681	H	GLY A	73	-12.778	8.789	16.067
ATOM	682	CA	GLY A	73	-11.253	9.755	14.938
ATOM	683	C	GLY A	73	-11.283	8.554	14.034
ATOM	684	O	GLY A	73	-12.211	7.706	14.006
ATOM	685	N	THR A	74	-10.247	8.428	13.182
ATOM	686	H	THR A	74	-9.471	9.055	13.250
ATOM	687	CA	THR A	74	-10.201	7.416	12.158
ATOM	688	C	THR A	74	-9.674	6.134	12.760
ATOM	689	O	THR A	74	-8.670	6.034	13.497
ATOM	690	CB	THR A	74	-9.298	7.895	11.048
ATOM	691	OG1	THR A	74	-9.910	9.019	10.441
ATOM	692	HG1	THR A	74	-9.335	9.362	9.698
ATOM	693	CG2	THR A	74	-9.088	6.823	9.946
ATOM	694	N	VAL A	75	-10.318	5.027	12.327
ATOM	695	H	VAL A	75	-11.066	5.114	11.669
ATOM	696	CA	VAL A	75	-9.968	3.717	12.778
ATOM	697	C	VAL A	75	-9.906	2.843	11.551
ATOM	698	O	VAL A	75	-10.803	2.807	10.681
ATOM	699	CB	VAL A	75	-11.044	3.250	13.737
ATOM	700	CG1	VAL A	75	-11.021	1.721	13.943
ATOM	701	CG2	VAL A	75	-10.915	4.019	15.034
ATOM	702	N	LEU A	76	-8.768	2.139	11.366
ATOM	703	H	LEU A	76	-8.002	2.260	11.998
ATOM	704	CA	LEU A	76	-8.566	1.183	10.276
ATOM	705	C	LEU A	76	-8.848	-0.211	10.808
ATOM	706	O	LEU A	76	-8.514	-0.582	11.958
ATOM	707	CB	LEU A	76	-7.103	1.270	9.798
ATOM	708	CG	LEU A	76	-6.608	2.684	9.443
ATOM	709	CD1	LEU A	76	-5.151	2.645	9.087
ATOM	710	CD2	LEU A	76	-7.396	3.302	8.296
ATOM	711	N	VAL A	77	-9.569	-1.062	10.042
ATOM	712	H	VAL A	77	-9.894	-0.766	9.144
ATOM	713	CA	VAL A	77	-9.899	-2.428	10.485
ATOM	714	C	VAL A	77	-9.298	-3.412	9.482
ATOM	715	O	VAL A	77	-9.450	-3.300	8.253
ATOM	716	CB	VAL A	77	-11.436	-2.592	10.506
ATOM	717	CG1	VAL A	77	-11.830	-4.021	10.682
ATOM	718	CG2	VAL A	77	-12.072	-1.765	11.634
ATOM	719	N	GLY A	78	-8.560	-4.402	9.928
ATOM	720	H	GLY A	78	-8.445	-4.530	10.913
ATOM	721	CA	GLY A	78	-7.930	-5.285	8.987
ATOM	722	C	GLY A	78	-7.228	-6.380	9.732
ATOM	723	O	GLY A	78	-7.292	-6.524	10.970
ATOM	724	N	PRO A	79	-6.512	-7.271	9.003
ATOM	725	CA	PRO A	79	-5.880	-8.467	9.602
ATOM	726	C	PRO A	79	-4.599	-8.107	10.340
ATOM	727	O	PRO A	79	-3.449	-8.489	10.032

FIG. I IM

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ATOM    728  CB   PRO A   79      -5.613   -9.379    8.400
ATOM    729  CG   PRO A   79      -5.529   -8.416    7.210
ATOM    730  CD   PRO A   79      -6.415   -7.225    7.537
ATOM    731  N    THR A   80      -4.759   -7.304   11.406
ATOM    732  H    THR A   80      -5.664   -6.935   11.619
ATOM    733  CA   THR A   80      -3.658   -6.957   12.263
ATOM    734  C    THR A   80      -3.490   -8.075   13.308
ATOM    735  O    THR A   80      -4.447   -8.642   13.857
ATOM    736  CB   THR A   80      -3.868   -5.572   12.927
ATOM    737  OG1  THR A   80      -2.770   -5.303   13.787
ATOM    738  HG1  THR A   80      -2.889   -4.412   14.225
ATOM    739  CG2  THR A   80      -5.210   -5.464   13.678
ATOM    740  N    PRO A   81      -2.243   -8.496   13.589
ATOM    741  CA   PRO A   81      -1.986   -9.476   14.660
ATOM    742  C    PRO A   81      -2.499   -8.952   16.001
ATOM    743  O    PRO A   81      -2.944   -9.720   16.866
ATOM    744  CB   PRO A   81      -0.444   -9.549   14.732
ATOM    745  CG   PRO A   81       0.069   -8.951   13.429
ATOM    746  CD   PRO A   81      -1.029   -8.105   12.842
ATOM    747  N    VAL A   82      -2.474   -7.621   16.276
ATOM    748  H    VAL A   82      -2.180   -6.975   15.571
ATOM    749  CA   VAL A   82      -2.869   -7.091   17.591
ATOM    750  C    VAL A   82      -3.605   -5.761   17.379
ATOM    751  O    VAL A   82      -3.349   -5.004   16.429
ATOM    752  CB   VAL A   82      -1.595   -6.858   18.443
ATOM    753  CG1  VAL A   82      -0.650   -5.824   17.803
ATOM    754  CG2  VAL A   82      -1.907   -6.418   19.890
ATOM    755  N    ASN A   83      -4.548   -5.371   18.260
ATOM    756  H    ASN A   83      -4.810   -5.981   19.007
ATOM    757  CA   ASN A   83      -5.181   -4.067   18.123
ATOM    758  C    ASN A   83      -4.195   -3.019   18.565
ATOM    759  O    ASN A   83      -3.605   -3.064   19.665
ATOM    760  CB   ASN A   83      -6.436   -3.942   18.982
ATOM    761  CG   ASN A   83      -7.502   -4.930   18.631
ATOM    762  OD1  ASN A   83      -7.899   -5.049   17.488
ATOM    763  ND2  ASN A   83      -7.980   -5.662   19.628
ATOM    764 2HD2  ASN A   83      -8.695   -6.341   19.459
ATOM    765 1HD2  ASN A   83      -7.630   -5.541   20.557
ATOM    766  N    ILE A   84      -4.007   -1.951   17.770
ATOM    767  H    ILE A   84      -4.583   -1.827   16.962
ATOM    768  CA   ILE A   84      -2.993   -0.954   18.032
ATOM    769  C    ILE A   84      -3.679    0.387   18.114
ATOM    770  O    ILE A   84      -4.460    0.797   17.240
ATOM    771  CB   ILE A   84      -2.021   -0.922   16.833
ATOM    772  CG1  ILE A   84      -1.162   -2.150   16.859
ATOM    773  CG2  ILE A   84      -1.219    0.387   16.747
ATOM    774  CD1  ILE A   84      -0.375   -2.360   15.579
ATOM    775  N    ILE A   85      -3.471    1.155   19.203
ATOM    776  H    ILE A   85      -2.972    0.781   19.985
ATOM    777  CA   ILE A   85      -3.951    2.518   19.281
ATOM    778  C    ILE A   85      -2.784    3.425   18.949
ATOM    779  O    ILE A   85      -1.767    3.515   19.663
ATOM    780  CB   ILE A   85      -4.522    2.825   20.676
ATOM    781  CG1  ILE A   85      -5.673    1.865   21.050
ATOM    782  CG2  ILE A   85      -5.000    4.274   20.716
ATOM    783  CD1  ILE A   85      -6.828    1.808   20.059
```

FIG. 1 IN

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ATOM	784	N	GLY A	86	-2.820	4.123	17.792
ATOM	785	H	GLY A	86	-3.637	4.087	17.217
ATOM	786	CA	GLY A	86	-1.690	4.936	17.351
ATOM	787	C	GLY A	86	-1.831	6.393	17.704
ATOM	788	O	GLY A	86	-2.760	6.864	18.390
ATOM	789	N	ARG A	87	-0.881	7.229	17.230
ATOM	790	H	ARG A	87	-0.204	6.890	16.577
ATOM	791	CA	ARG A	87	-0.810	8.623	17.643
ATOM	792	C	ARG A	87	-2.027	9.445	17.277
ATOM	793	O	ARG A	87	-2.365	10.430	17.963
ATOM	794	CB	ARG A	87	0.450	9.275	17.057
ATOM	795	CG	ARG A	87	1.735	8.496	17.205
ATOM	796	CD	ARG A	87	2.762	8.916	16.207
ATOM	797	NE	ARG A	87	3.875	7.961	16.117
ATOM	798	HE	ARG A	87	4.035	7.353	16.895
ATOM	799	CZ	ARG A	87	4.660	7.893	15.035
ATOM	800	NH1	ARG A	87	4.463	8.675	13.975
ATOM	801	2HH1	ARG A	87	3.712	9.335	13.974
ATOM	802	1HH1	ARG A	87	5.066	8.602	13.181
ATOM	803	NH2	ARG A	87	5.656	7.019	15.023
ATOM	804	1HH2	ARG A	87	6.254	6.953	14.224
ATOM	805	2HH2	ARG A	87	5.810	6.426	15.813
ATOM	806	N	ASN A	88	-2.780	9.120	16.214
ATOM	807	H	ASN A	88	-2.504	8.361	15.625
ATOM	808	CA	ASN A	88	-4.015	9.860	15.890
ATOM	809	C	ASN A	88	-4.963	9.921	17.069
ATOM	810	O	ASN A	88	-5.613	10.954	17.345
ATOM	811	CB	ASN A	88	-4.712	9.315	14.617
ATOM	812	CG	ASN A	88	-5.475	8.001	14.827
ATOM	813	OD1	ASN A	88	-4.922	6.996	15.245
ATOM	814	ND2	ASN A	88	-6.758	7.998	14.506
ATOM	815	2HD2	ASN A	88	-7.306	7.169	14.622
ATOM	816	1HD2	ASN A	88	-7.190	8.824	14.145
ATOM	817	N	LEU A	89	-5.130	8.847	17.848
ATOM	818	H	LEU A	89	-4.637	8.002	17.640
ATOM	819	CA	LEU A	89	-6.024	8.865	19.013
ATOM	820	C	LEU A	89	-5.275	9.091	20.309
ATOM	821	O	LEU A	89	-5.834	9.632	21.283
ATOM	822	CB	LEU A	89	-6.840	7.592	19.140
ATOM	823	CG	LEU A	89	-7.759	7.355	17.957
ATOM	824	CD1	LEU A	89	-8.369	5.980	18.088
ATOM	825	CD2	LEU A	89	-8.817	8.457	17.801
ATOM	826	N	LEU A	90	-3.983	8.745	20.428
ATOM	827	H	LEU A	90	-3.525	8.274	19.674
ATOM	828	CA	LEU A	90	-3.242	9.057	21.664
ATOM	829	C	LEU A	90	-3.155	10.555	21.932
ATOM	830	O	LEU A	90	-3.202	11.020	23.092
ATOM	831	CB	LEU A	90	-1.817	8.453	21.661
ATOM	832	CG	LEU A	90	-1.766	6.914	21.587
ATOM	833	CD1	LEU A	90	-0.343	6.494	21.396
ATOM	834	CD2	LEU A	90	-2.339	6.230	22.812
ATOM	835	N	THR A	91	-3.031	11.407	20.926
ATOM	836	H	THR A	91	-2.982	11.063	19.988
ATOM	837	CA	THR A	91	-2.964	12.834	21.155
ATOM	838	C	THR A	91	-4.309	13.331	21.635
ATOM	839	O	THR A	91	-4.422	14.315	22.398

FIG. 110

ATOM	840	CB	THR A	91	-2.555	13.543	19.848
ATOM	841	OG1	THR A	91	-3.459	13.214	18.802
ATOM	842	HG1	THR A	91	-3.188	13.677	17.958
ATOM	843	CG2	THR A	91	-1.153	13.122	19.395
ATOM	844	N	GLN A	92	-5.435	12.704	21.258
ATOM	845	H	GLN A	92	-5.379	11.892	20.677
ATOM	846	CA	GLN A	92	-6.763	13.186	21.682
ATOM	847	C	GLN A	92	-6.942	12.975	23.153
ATOM	848	O	GLN A	92	-7.554	13.797	23.871
ATOM	849	CB	GLN A	92	-7.890	12.479	20.964
ATOM	850	CG	GLN A	92	-7.937	12.862	19.517
ATOM	851	CD	GLN A	92	-9.251	12.515	18.886
ATOM	852	OE1	GLN A	92	-10.270	12.424	19.546
ATOM	853	NE2	GLN A	92	-9.202	12.323	17.588
ATOM	854	1HE2	GLN A	92	-10.031	12.087	17.080
ATOM	855	2HE2	GLN A	92	-8.336	12.411	17.097
ATOM	856	N	ILE A	93	-6.472	11.846	23.721
ATOM	857	H	ILE A	93	-6.014	11.160	23.155
ATOM	858	CA	ILE A	93	-6.608	11.578	25.165
ATOM	859	C	ILE A	93	-5.472	12.189	25.948
ATOM	860	O	ILE A	93	-5.342	12.031	27.171
ATOM	861	CB	ILE A	93	-6.820	10.073	25.484
ATOM	862	CG1	ILE A	93	-5.536	9.221	25.286
ATOM	863	CG2	ILE A	93	-8.022	9.486	24.735
ATOM	864	CD1	ILE A	93	-5.754	7.740	25.693
ATOM	865	N	GLY A	94	-4.594	12.993	25.330
ATOM	866	H	GLY A	94	-4.617	13.079	24.334
ATOM	867	CA	GLY A	94	-3.613	13.742	26.063
ATOM	868	C	GLY A	94	-2.448	12.895	26.512
ATOM	869	O	GLY A	94	-1.764	13.158	27.519
ATOM	870	N	CYS A	95	-2.117	11.849	25.797
ATOM	871	H	CYS A	95	-2.619	11.644	24.957
ATOM	872	CA	CYS A	95	-1.036	10.994	26.214
ATOM	873	C	CYS A	95	0.362	11.566	25.925
ATOM	874	O	CYS A	95	0.588	12.254	24.907
ATOM	875	CB	CYS A	95	-1.260	9.655	25.550
ATOM	876	SG	CYS A	95	-0.254	8.307	26.125
ATOM	877	N	THR A	96	1.346	11.297	26.803
ATOM	878	H	THR A	96	1.135	10.738	27.618
ATOM	879	CA	THR A	96	2.728	11.779	26.664
ATOM	880	C	THR A	96	3.729	10.784	27.264
ATOM	881	O	THR A	96	3.498	10.249	28.345
ATOM	882	CB	THR A	96	2.925	13.154	27.346
ATOM	883	OG1	THR A	96	2.594	13.109	28.721
ATOM	884	HG1	THR A	96	2.784	13.966	29.109
ATOM	885	CG2	THR A	96	2.139	14.300	26.698
ATOM	886	N	LEU A	97	4.882	10.603	26.599
ATOM	887	H	LEU A	97	5.016	11.071	25.714
ATOM	888	CA	LEU A	97	6.040	9.910	27.166
ATOM	889	C	LEU A	97	6.751	10.824	28.175
ATOM	890	O	LEU A	97	6.705	12.046	28.044
ATOM	891	CB	LEU A	97	7.013	9.497	26.049
ATOM	892	CG	LEU A	97	6.452	8.449	25.065
ATOM	893	CD1	LEU A	97	7.360	8.355	23.828
ATOM	894	CD2	LEU A	97	6.345	7.065	25.724
ATOM	895	N	ASN A	98	7.412	10.221	29.175

FIG. I IP

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ATOM    896    H     ASN A  98        7.413    9.212   29.205
ATOM    897    CA    ASN A  98        8.065   10.897   30.292
ATOM    898    C     ASN A  98        9.220   10.029   30.800
ATOM    899    O     ASN A  98        8.995    9.079   31.550
ATOM    900    CB    ASN A  98        7.057   11.177   31.423
ATOM    901    CG    ASN A  98        6.084   12.305   31.083
ATOM    902    OD1   ASN A  98        4.983   12.062   30.594
ATOM    903    ND2   ASN A  98        6.493   13.549   31.342
ATOM    904   2HD2   ASN A  98        5.888   14.331   31.136
ATOM    905   1HD2   ASN A  98       ·7.406   13.707   31.742
ATOM    906    N     LEU A  99       10.451   10.369   30.389
ATOM    907    H     LEU A  99       10.547   11.177   29.792
ATOM    908    CA    LEU A  99       11.679    9.620   30.666
ATOM    909    C     LEU A  99       12.711   10.437   31.454
ATOM    910    O     LEU A  99       12.487   11.652   31.651
ATOM    911    CB    LEU A  99       12.233    8.989   29.369
ATOM    912    CG    LEU A  99       12.833    9.873   28.248
ATOM    913    CD1   LEU A  99       11.876   10.947   27.705
ATOM    914    CD2   LEU A  99       14.183   10.505   28.623
ATOM    915    OXT   LEU A  99       13.716    9.819   31.869
TER
ATOM    916    N     PRO B   1       12.600   14.237   30.106
ATOM    917    CA    PRO B   1       11.842   15.268   29.363
ATOM    918    C     PRO B   1       10.430   14.773   29.138
ATOM    919    O     PRO B   1       10.054   13.695   29.618
ATOM    920    CB    PRO B   1       12.622   15.412   28.035
ATOM    921    CG    PRO B   1       13.817   14.470   28.131
ATOM    922    CD    PRO B   1       13.966   14.227   29.603
ATOM    923   1H     PRO B   1       12.175   13.343   29.964
ATOM    924   2H     PRO B   1       12.594   14.457   31.081
ATOM    925    N     GLN B   2        9.513   15.542   28.523
ATOM    926    H     GLN B   2        9.751   16.474   28.251
ATOM    927    CA    GLN B   2        8.186   15.058   28.242
ATOM    928    C     GLN B   2        8.066   15.151   26.749
ATOM    929    O     GLN B   2        8.523   16.140   26.133
ATOM    930    CB    GLN B   2        7.155   15.976   28.856
ATOM    931    CG    GLN B   2        5.739   15.732   28.373
ATOM    932    CD    GLN B   2        4.744   16.365   29.284
ATOM    933    OE1   GLN B   2        4.628   15.962   30.431
ATOM    934    NE2   GLN B   2        4.024   17.367   28.784
ATOM    935   1HE2   GLN B   2        3.341   17.830   29.349
ATOM    936   2HE2   GLN B   2        4.160   17.665   27.839
ATOM    937    N     ILE B   3        7.499   14.176   26.036
ATOM    938    H     ILE B   3        7.102   13.386   26.504
ATOM    939    CA    ILE B   3        7.435   14.216   24.601
ATOM    940    C     ILE B   3        5.956   14.097   24.184
ATOM    941    O     ILE B   3        5.150   13.290   24.710
ATOM    942    CB    ILE B   3        8.299   13.058   24.029
ATOM    943    CG1   ILE B   3        9.743   13.232   24.534
ATOM    944    CG2   ILE B   3        8.269   12.985   22.496
ATOM    945    CD1   ILE B   3       10.621   12.068   24.143
ATOM    946    N     THR B   4        5.462   15.108   23.453
ATOM    947    H     THR B   4        6.046   15.887   23.226
ATOM    948    CA    THR B   4        4.107   15.115   22.976
ATOM    949    C     THR B   4        4.039   14.193   21.765
ATOM    950    O     THR B   4        5.066   13.755   21.203
```

FIG. 11Q

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ATOM	951	CB	THR	B	4	3.616	16.548	22.647
ATOM	952	OG1	THR	B	4	4.450	17.157	21.645
ATOM	953	HG1	THR	B	4	4.123	18.080	21.442
ATOM	954	CG2	THR	B	4	3.644	17.454	23.876
ATOM	955	N	LEU	B	5	2.872	13.781	21.324
ATOM	956	H	LEU	B	5	2.033	14.151	21.723
ATOM	957	CA	LEU	B	5	2.837	12.795	20.265
ATOM	958	C	LEU	B	5	2.183	13.415	19.047
ATOM	959	O	LEU	B	5	1.677	12.720	18.142
ATOM	960	CB	LEU	B	5	2.093	11.577	20.762
ATOM	961	CG	LEU	B	5	2.819	10.856	21.892
ATOM	962	CD1	LEU	B	5	1.889	9.885	22.602
ATOM	963	CD2	LEU	B	5	4.108	10.159	21.416
ATOM	964	N	TRP	B	6	2.209	14.742	18.880
ATOM	965	H	TRP	B	6	2.601	15.323	19.593
ATOM	966	CA	TRP	B	6	1.683	15.364	17.690
ATOM	967	C	TRP	B	6	2.581	14.978	16.509
ATOM	968	O	TRP	B	6	2.159	14.851	15.349
ATOM	969	CB	TRP	B	6	1.587	16.879	17.833
ATOM	970	CG	TRP	B	6	0.652	17.339	18.921
ATOM	971	CD1	TRP	B	6	0.955	17.584	20.232
ATOM	972	CD2	TRP	B	6	-0.750	17.612	18.783
ATOM	973	NE1	TRP	B	6	-0.167	17.989	20.913
ATOM	974	HE1	TRP	B	6	-0.217	18.230	21.882
ATOM	975	CE2	TRP	B	6	-1.224	18.013	20.048
ATOM	976	CE3	TRP	B	6	-1.637	17.550	17.709
ATOM	977	CZ2	TRP	B	6	-2.544	18.352	20.266
ATOM	978	CZ3	TRP	B	6	-2.947	17.885	17.921
ATOM	979	CH2	TRP	B	6	-3.394	18.281	19.185
ATOM	980	N	GLN	B	7	3.896	14.809	16.738
ATOM	981	H	GLN	B	7	4.267	14.985	17.650
ATOM	982	CA	GLN	B	7	4.794	14.376	15.689
ATOM	983	C	GLN	B	7	5.361	13.043	16.096
ATOM	984	O	GLN	B	7	5.221	12.586	17.243
ATOM	985	CB	GLN	B	7	5.880	15.430	15.505
ATOM	986	CG	GLN	B	7	5.353	16.704	14.804
ATOM	987	CD	GLN	B	7	6.197	17.912	15.137
ATOM	988	OE1	GLN	B	7	7.400	17.802	15.404
ATOM	989	NE2	GLN	B	7	5.553	19.083	15.121
ATOM	990	1HE2	GLN	B	7	6.040	19.931	15.330
ATOM	991	2HE2	GLN	B	7	4.579	19.121	14.900
ATOM	992	N	ARG	B	8	5.979	12.274	15.189
ATOM	993	H	ARG	B	8	6.073	12.597	14.247
ATOM	994	CA	ARG	B	8	6.505	10.985	15.573
ATOM	995	C	ARG	B	8	7.577	11.198	16.610
ATOM	996	O	ARG	B	8	8.395	12.130	16.515
ATOM	997	CB	ARG	B	8	7.092	10.238	14.384
ATOM	998	CG	ARG	B	8	6.132	10.018	13.237
ATOM	999	CD	ARG	B	8	6.802	9.402	12.046
ATOM	1000	NE	ARG	B	8	5.846	9.005	11.023
ATOM	1001	HE	ARG	B	8	4.872	9.080	11.237
ATOM	1002	CZ	ARG	B	8	6.217	8.552	9.828
ATOM	1003	NH1	ARG	B	8	7.496	8.442	9.486
ATOM	1004	2HH1	ARG	B	8	8.211	8.703	10.134
ATOM	1005	1HH1	ARG	B	8	7.744	8.098	8.580
ATOM	1006	NH2	ARG	B	8	5.279	8.202	8.952

FIG. 1 IR

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ATOM	1007	1HH2	ARG	B	8	5.540	7.860	8.050
ATOM	1008	2HH2	ARG	B	8	4.312	8.281	9.196
ATOM	1009	N	PRO	B	9	7.663	10.381	17.682
ATOM	1010	CA	PRO	B	9	8.666	10.587	18.746
ATOM	1011	C	PRO	B	9	10.065	10.196	18.315
ATOM	1012	O	PRO	B	9	10.678	9.215	18.778
ATOM	1013	CB	PRO	B	9	8.148	9.682	19.878
ATOM	1014	CG	PRO	B	9	7.315	8.607	19.206
ATOM	1015	CD	PRO	B	9	6.708	9.323	18.004
ATOM	1016	N	LEU	B	10	10.685	10.969	17.400
ATOM	1017	H	LEU	B	10	10.201	11.746	16.998
ATOM	1018	CA	LEU	B	10	12.040	10.706	16.978
ATOM	1019	C	LEU	B	10	12.976	11.498	17.850
ATOM	1020	O	LEU	B	10	12.880	12.733	18.018
ATOM	1021	CB	LEU	B	10	12.250	11.170	15.554
ATOM	1022	CG	LEU	B	10	11.427	10.386	14.551
ATOM	1023	CD1	LEU	B	10	11.385	11.175	13.276
ATOM	1024	CD2	LEU	B	10	11.956	8.947	14.355
ATOM	1025	N	VAL	B	11	14.030	10.843	18.384
ATOM	1026	H	VAL	B	11	14.148	9.866	18.206
ATOM	1027	CA	VAL	B	11	15.018	11.517	19.223
ATOM	1028	C	VAL	B	11	16.400	11.111	18.740
ATOM	1029	O	VAL	B	11	16.581	10.201	17.911
ATOM	1030	CB	VAL	B	11	14.857	11.100	20.699
ATOM	1031	CG1	VAL	B	11	13.514	11.586	21.293
ATOM	1032	CG2	VAL	B	11	15.038	9.573	20.903
ATOM	1033	N	THR	B	12	17.485	11.739	19.232
ATOM	1034	H	THR	B	12	17.370	12.507	19.862
ATOM	1035	CA	THR	B	12	18.843	11.325	18.868
ATOM	1036	C	THR	B	12	19.377	10.284	19.837
ATOM	1037	O	THR	B	12	19.237	10.352	21.082
ATOM	1038	CB	THR	B	12	19.830	12.520	18.820
ATOM	1039	OG1	THR	B	12	19.389	13.483	17.876
ATOM	1040	HG1	THR	B	12	20.028	14.252	17.848
ATOM	1041	CG2	THR	B	12	21.234	12.075	18.399
ATOM	1042	N	ILE	B	13	20.044	9.234	19.338
ATOM	1043	H	ILE	B	13	20.135	9.130	18.348
ATOM	1044	CA	ILE	B	13	20.641	8.239	20.176
ATOM	1045	C	ILE	B	13	22.119	8.226	19.855
ATOM	1046	O	ILE	B	13	22.579	8.817	18.865
ATOM	1047	CB	ILE	B	13	19.993	6.870	19.879
ATOM	1048	CG1	ILE	B	13	20.192	6.464	18.415
ATOM	1049	CG2	ILE	B	13	18.482	6.893	20.206
ATOM	1050	CD1	ILE	B	13	19.829	5.035	18.106
ATOM	1051	N	LYS	B	14	22.973	7.618	20.661
ATOM	1052	H	LYS	B	14	22.652	7.243	21.531
ATOM	1053	CA	LYS	B	14	24.364	7.480	20.317
ATOM	1054	C	LYS	B	14	24.680	6.029	20.477
ATOM	1055	O	LYS	B	14	24.353	5.353	21.484
ATOM	1056	CB	LYS	B	14	25.266	8.263	21.242
ATOM	1057	CG	LYS	B	14	24.947	9.729	21.236
ATOM	1058	CD	LYS	B	14	25.664	10.498	22.339
ATOM	1059	CE	LYS	B	14	26.758	11.441	21.807
ATOM	1060	NZ	LYS	B	14	28.026	10.781	21.440
ATOM	1061	1HZ	LYS	B	14	28.674	11.466	21.107
ATOM	1062	3HZ	LYS	B	14	27.855	10.107	20.722

FIG. 1 IS

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ATOM    1063  2HZ   LYS B  14      28.408   10.323   22.243
ATOM    1064   N    ILE B  15      25.214    5.390   19.425
ATOM    1065   H    ILE B  15      25.434    5.901   18.594
ATOM    1066   CA   ILE B  15      25.489    3.989   19.434
ATOM    1067   C    ILE B  15      26.832    3.981   18.750
ATOM    1068   O    ILE B  15      27.104    4.869   17.933
ATOM    1069   CB   ILE B  15      24.435    3.220   18.606
ATOM    1070   CG1  ILE B  15      24.893    1.824   18.347
ATOM    1071   CG2  ILE B  15      24.048    3.977   17.309
ATOM    1072   CD1  ILE B  15      23.830    0.996   17.645
ATOM    1073   N    GLY B  16      27.812    3.212   19.202
ATOM    1074   H    GLY B  16      27.623    2.535   19.913
ATOM    1075   CA   GLY B  16      29.175    3.336   18.677
ATOM    1076   C    GLY B  16      29.771    4.754   18.619
ATOM    1077   O    GLY B  16      30.737    4.970   17.902
ATOM    1078   N    GLY B  17      29.273    5.791   19.335
ATOM    1079   H    GLY B  17      28.453    5.660   19.892
ATOM    1080   CA   GLY B  17      29.924    7.105   19.302
ATOM    1081   C    GLY B  17      29.468    8.043   18.176
ATOM    1082   O    GLY B  17      29.984    9.155   17.933
ATOM    1083   N    GLN B  18      28.433    7.621   17.411
ATOM    1084   H    GLN B  18      28.046    6.711   17.560
ATOM    1085   CA   GLN B  18      27.834    8.449   16.348
ATOM    1086   C    GLN B  18      26.407    8.755   16.736
ATOM    1087   O    GLN B  18      25.678    7.953   17.353
ATOM    1088   CB   GLN B  18      27.810    7.645   15.045
ATOM    1089   CG   GLN B  18      27.247    6.204   15.146
ATOM    1090   CD   GLN B  18      27.572    5.333   13.924
ATOM    1091   OE1  GLN B  18      26.771    4.501   13.464
ATOM    1092   NE2  GLN B  18      28.766    5.531   13.393
ATOM    1093  1HE2  GLN B  18      29.057    5.005   12.594
ATOM    1094  2HE2  GLN B  18      29.388    6.209   13.786
ATOM    1095   N    LEU B  19      25.873    9.933   16.337
ATOM    1096   H    LEU B  19      26.446   10.602   15.863
ATOM    1097   CA   LEU B  19      24.467   10.267   16.578
ATOM    1098   C    LEU B  19      23.633    9.622   15.490
ATOM    1099   O    LEU B  19      23.912    9.707   14.284
ATOM    1100   CB   LEU B  19      24.207   11.777   16.457
ATOM    1101   CG   LEU B  19      24.857   12.756   17.454
ATOM    1102   CD1  LEU B  19      24.739   12.335   18.880
ATOM    1103   CD2  LEU B  19      26.299   13.072   17.130
ATOM    1104   N    LYS B  20      22.450    9.085   15.850
ATOM    1105   H    LYS B  20      22.242    8.948   16.819
ATOM    1106   CA   LYS B  20      21.472    8.702   14.867
ATOM    1107   C    LYS B  20      20.121    9.105   15.417
ATOM    1108   O    LYS B  20      19.957    9.572   16.569
ATOM    1109   CB   LYS B  20      21.496    7.200   14.560
ATOM    1110   CG   LYS B  20      22.904    6.653   14.507
ATOM    1111   CD   LYS B  20      23.052    5.366   13.677
ATOM    1112   CE   LYS B  20      23.069    5.603   12.145
ATOM    1113   NZ   LYS B  20      23.893    6.758   11.699
ATOM    1114  1HZ   LYS B  20      23.847    6.836   10.703
ATOM    1115  3HZ   LYS B  20      24.843    6.617   11.978
ATOM    1116  2HZ   LYS B  20      23.544    7.597   12.116
ATOM    1117   N    GLU B  21      19.068    9.022   14.591
ATOM    1118   H    GLU B  21      19.200    8.712   13.650
```

FIG. 1 IT

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ATOM	1119	CA	GLU	B	21	17.735	9.366	15.008
ATOM	1120	C	GLU	B	21	16.937	8.095	15.119
ATOM	1121	O	GLU	B	21	17.117	7.103	14.376
ATOM	1122	CB	GLU	B	21	17.143	10.314	13.983
ATOM	1123	CG	GLU	B	21	15.714	10.706	14.162
ATOM	1124	CD	GLU	B	21	15.304	11.607	13.036
ATOM	1125	OE1	GLU	B	21	14.971	11.051	11.957
ATOM	1126	OE2	GLU	B	21	15.338	12.854	13.174
ATOM	1127	N	ALA	B	22	16.025	7.999	16.072
ATOM	1128	H	ALA	B	22	15.825	8.792	16.648
ATOM	1129	CA	ALA	B	22	15.300	6.783	16.315
ATOM	1130	C	ALA	B	22	13.981	7.132	16.952
ATOM	1131	O	ALA	B	22	13.756	8.153	17.632
ATOM	1132	CB	ALA	B	22	16.095	5.865	17.235
ATOM	1133	N	LEU	B	23	12.994	6.230	16.743
ATOM	1134	H	LEU	B	23	13.195	5.379	16.257
ATOM	1135	CA	LEU	B	23	11.639	6.408	17.180
ATOM	1136	C	LEU	B	23	11.476	5.740	18.534
ATOM	1137	O	LEU	B	23	11.814	4.564	18.746
ATOM	1138	CB	LEU	B	23	10.775	5.665	16.192
ATOM	1139	CG	LEU	B	23	9.267	5.810	16.237
ATOM	1140	CD1	LEU	B	23	8.807	7.142	15.664
ATOM	1141	CD2	LEU	B	23	8.648	4.625	15.482
ATOM	1142	N	LEU	B	24	10.948	6.455	19.553
ATOM	1143	H	LEU	B	24	10.775	7.433	19.435
ATOM	1144	CA	LEU	B	24	10.613	5.838	20.849
ATOM	1145	C	LEU	B	24	9.271	5.160	20.687
ATOM	1146	O	LEU	B	24	8.208	5.764	20.418
ATOM	1147	CB	LEU	B	24	10.564	6.878	21.971
ATOM	1148	CG	LEU	B	24	11.828	7.750	22.075
ATOM	1149	CD1	LEU	B	24	11.580	8.859	23.077
ATOM	1150	CD2	LEU	B	24	13.099	6.955	22.388
ATOM	1151	N	ASP	B	25	9.246	3.822	20.809
ATOM	1152	H	ASP	B	25	10.025	3.347	21.218
ATOM	1153	CA	ASP	B	25	8.122	3.030	20.366
ATOM	1154	C	ASP	B	25	7.637	2.136	21.484
ATOM	1155	O	ASP	B	25	8.189	1.048	21.759
ATOM	1156	CB	ASP	B	25	8.613	2.196	19.189
ATOM	1157	CG	ASP	B	25	7.528	1.421	18.511
ATOM	1158	OD1	ASP	B	25	6.422	1.339	19.058
ATOM	1159	OD2	ASP	B	25	7.800	0.897	17.426
ATOM	1160	N	THR	B	26	6.547	2.465	22.157
ATOM	1161	H	THR	B	26	6.067	3.314	21.938
ATOM	1162	CA	THR	B	26	6.025	1.621	23.212
ATOM	1163	C	THR	B	26	5.347	0.369	22.694
ATOM	1164	O	THR	B	26	4.976	-0.550	23.451
ATOM	1165	CB	THR	B	26	5.027	2.389	24.046
ATOM	1166	OG1	THR	B	26	3.927	2.853	23.239
ATOM	1167	HG1	THR	B	26	3.277	3.359	23.806
ATOM	1168	CG2	THR	B	26	5.703	3.603	24.650
ATOM	1169	N	GLY	B	27	5.090	0.245	21.382
ATOM	1170	H	GLY	B	27	5.341	0.983	20.756
ATOM	1171	CA	GLY	B	27	4.457	-0.938	20.867
ATOM	1172	C	GLY	B	27	5.475	-1.992	20.458
ATOM	1173	O	GLY	B	27	5.121	-3.108	20.055
ATOM	1174	N	ALA	B	28	6.792	-1.717	20.495

FIG. 1 IU

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ATOM	1175	H	ALA	B	28	7.104	-0.832	20.841
ATOM	1176	CA	ALA	B	28	7.800	-2.690	20.037
ATOM	1177	C	ALA	B	28	8.371	-3.444	21.259
ATOM	1178	O	ALA	B	28	8.840	-2.807	22.213
ATOM	1179	CB	ALA	B	28	8.924	-1.936	19.358
ATOM	1180	N	ASP	B	29	8.459	-4.787	21.289
ATOM	1181	H	ASP	B	29	8.082	-5.325	20.535
ATOM	1182	CA	ASP	B	29	9.121	-5.441	22.452
ATOM	1183	C	ASP	B	29	10.608	-5.219	22.404
ATOM	1184	O	ASP	B	29	11.345	-5.264	23.412
ATOM	1185	CB	ASP	B	29	8.965	-6.975	22.447
ATOM	1186	CG	ASP	B	29	7.551	-7.477	22.774
ATOM	1187	OD1	ASP	B	29	6.683	-6.693	23.169
ATOM	1188	OD2	ASP	B	29	7.350	-8.686	22.616
ATOM	1189	N	ASP	B	30	11.164	-5.157	21.171
ATOM	1190	H	ASP	B	30	10.577	-5.063	20.367
ATOM	1191	CA	ASP	B	30	12.609	-5.217	20.880
ATOM	1192	C	ASP	B	30	13.048	-3.886	20.335
ATOM	1193	O	ASP	B	30	12.269	-3.055	19.817
ATOM	1194	CB	ASP	B	30	12.833	-6.226	19.735
ATOM	1195	CG	ASP	B	30	12.477	-7.675	20.099
ATOM	1196	OD1	ASP	B	30	13.197	-8.272	20.908
ATOM	1197	OD2	ASP	B	30	11.494	-8.237	19.569
ATOM	1198	N	THR	B	31	14.387	-3.692	20.227
ATOM	1199	H	THR	B	31	15.018	-4.380	20.586
ATOM	1200	CA	THR	B	31	14.981	-2.530	19.614
ATOM	1201	C	THR	B	31	15.578	-2.979	18.260
ATOM	1202	O	THR	B	31	16.246	-4.020	18.123
ATOM	1203	CB	THR	B	31	16.036	-2.004	20.557
ATOM	1204	OG1	THR	B	31	15.378	-1.376	21.645
ATOM	1205	HG1	THR	B	31	16.052	-1.016	22.290
ATOM	1206	CG2	THR	B	31	16.944	-0.960	19.904
ATOM	1207	N	VAL	B	32	15.237	-2.283	17.150
ATOM	1208	H	VAL	B	32	14.703	-1.442	17.237
ATOM	1209	CA	VAL	B	32	15.626	-2.722	15.806
ATOM	1210	C	VAL	B	32	16.303	-1.566	15.132
ATOM	1211	O	VAL	B	32	15.779	-0.428	14.995
ATOM	1212	CB	VAL	B	32	14.407	-3.126	14.964
ATOM	1213	CG1	VAL	B	32	14.820	-3.703	13.596
ATOM	1214	CG2	VAL	B	32	13.556	-4.102	15.703
ATOM	1215	N	LEU	B	33	17.563	-1.756	14.720
ATOM	1216	H	LEU	B	33	17.984	-2.658	14.814
ATOM	1217	CA	LEU	B	33	18.347	-0.697	14.138
ATOM	1218	C	LEU	B	33	18.610	-1.009	12.685
ATOM	1219	O	LEU	B	33	18.685	-2.162	12.205
ATOM	1220	CB	LEU	B	33	19.679	-0.628	14.856
ATOM	1221	CG	LEU	B	33	19.698	0.363	16.031
ATOM	1222	CD1	LEU	B	33	18.425	0.321	16.891
ATOM	1223	CD2	LEU	B	33	20.929	0.179	16.889
ATOM	1224	N	GLU	B	34	18.786	0.078	11.899
ATOM	1225	H	GLU	B	34	18.619	0.991	12.271
ATOM	1226	CA	GLU	B	34	19.218	0.041	10.488
ATOM	1227	C	GLU	B	34	20.478	-0.774	10.399
ATOM	1228	O	GLU	B	34	21.374	-0.835	11.272
ATOM	1229	CB	GLU	B	34	19.536	1.460	9.996
ATOM	1230	CG	GLU	B	34	20.722	2.088	10.761

FIG. 1 IV

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ATOM   1231   CD   GLU B  34     21.085    3.512   10.314
ATOM   1232   OE1  GLU B  34     20.285    4.466   10.500
ATOM   1233   OE2  GLU B  34     22.211    3.703    9.775
ATOM   1234   N    GLU B  35     20.673   -1.367    9.205
ATOM   1235   H    GLU B  35     20.011   -1.227    8.468
ATOM   1236   CA   GLU B  35     21.802   -2.205    8.930
ATOM   1237   C    GLU B  35     23.096   -1.520    9.321
ATOM   1238   O    GLU B  35     23.391   -0.379    8.916
ATOM   1239   CB   GLU B  35     21.741   -2.479    7.439
ATOM   1240   CG   GLU B  35     22.795   -3.380    6.883
ATOM   1241   CD   GLU B  35     22.987   -4.587    7.744
ATOM   1242   OE1  GLU B  35     21.980   -5.258    8.118
ATOM   1243   OE2  GLU B  35     24.149   -4.860    8.048
ATOM   1244   N    MET B  36     23.926   -2.106   10.157
ATOM   1245   H    MET B  36     23.654   -2.953   10.613
ATOM   1246   CA   MET B  36     25.232   -1.559   10.441
ATOM   1247   C    MET B  36     26.146   -2.687   10.815
ATOM   1248   O    MET B  36     25.731   -3.783   11.257
ATOM   1249   CB   MET B  36     25.251   -0.424   11.497
ATOM   1250   CG   MET B  36     24.626   -0.724   12.881
ATOM   1251   SD   MET B  36     24.722    0.719   13.988
ATOM   1252   CE   MET B  36     23.132    1.586   13.692
ATOM   1253   N    SER B  37     27.441   -2.551   10.593
ATOM   1254   H    SER B  37     27.783   -1.726   10.144
ATOM   1255   CA   SER B  37     28.321   -3.608   11.011
ATOM   1256   C    SER B  37     28.721   -3.352   12.442
ATOM   1257   O    SER B  37     29.402   -2.369   12.788
ATOM   1258   CB   SER B  37     29.567   -3.622   10.109
ATOM   1259   OG   SER B  37     29.231   -3.908    8.750
ATOM   1260   HG   SER B  37     30.057   -3.911    8.187
ATOM   1261   N    LEU B  38     28.469   -4.295   13.366
ATOM   1262   H    LEU B  38     27.948   -5.123   13.117
ATOM   1263   CA   LEU B  38     29.073   -4.232   14.714
ATOM   1264   C    LEU B  38     30.132   -5.342   14.895
ATOM   1265   O    LEU B  38     30.070   -6.357   14.197
ATOM   1266   CB   LEU B  38     27.986   -4.237   15.802
ATOM   1267   CG   LEU B  38     27.005   -3.039   15.750
ATOM   1268   CD1  LEU B  38     25.885   -3.214   16.788
ATOM   1269   CD2  LEU B  38     27.707   -1.696   16.017
ATOM   1270   N    PRO B  39     31.119   -5.160   15.804
ATOM   1271   CA   PRO B  39     32.199   -6.116   16.052
ATOM   1272   C    PRO B  39     31.767   -7.223   17.028
ATOM   1273   O    PRO B  39     31.448   -6.942   18.185
ATOM   1274   CB   PRO B  39     33.347   -5.276   16.625
ATOM   1275   CG   PRO B  39     32.634   -4.148   17.370
ATOM   1276   CD   PRO B  39     31.385   -3.916   16.523
ATOM   1277   N    GLY B  40     31.770   -8.481   16.559
ATOM   1278   H    GLY B  40     32.036   -8.641   15.598
ATOM   1279   CA   GLY B  40     31.420   -9.658   17.353
ATOM   1280   C    GLY B  40     30.679  -10.723   16.539
ATOM   1281   O    GLY B  40     30.647  -10.671   15.308
ATOM   1282   N    LYS B  41     30.098  -11.699   17.255
ATOM   1283   H    LYS B  41     30.164  -11.656   18.261
ATOM   1284   CA   LYS B  41     29.399  -12.861   16.702
ATOM   1285   C    LYS B  41     27.971  -12.923   17.245
ATOM   1286   O    LYS B  41     27.743  -12.700   18.436
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FIG. I IW

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ATOM	1287	CB	LYS B	41	30.154	-14.152	17.048
ATOM	1288	CG	LYS B	41	31.537	-14.221	16.384
ATOM	1289	CD	LYS B	41	32.192	-15.508	16.651
ATOM	1290	CE	LYS B	41	33.566	-15.642	15.983
ATOM	1291	NZ	LYS B	41	34.198	-16.956	16.183
ATOM	1292	1HZ	LYS B	41	35.102	-16.968	15.732
ATOM	1293	3HZ	LYS B	41	33.612	-17.674	15.782
ATOM	1294	2HZ	LYS B	41	34.312	-17.128	17.172
ATOM	1295	N	TRP B	42	27.018	-13.228	16.351
ATOM	1296	H	TRP B	42	27.307	-13.458	15.411
ATOM	1297	CA	TRP B	42	25.597	-12.929	16.521
ATOM	1298	C	TRP B	42	24.723	-14.179	16.405
ATOM	1299	O	TRP B	42	25.210	-15.277	16.131
ATOM	1300	CB	TRP B	42	25.192	-11.856	15.491
ATOM	1301	CG	TRP B	42	26.127	-10.687	15.390
ATOM	1302	CD1	TRP B	42	26.651	-10.197	14.244
ATOM	1303	CD2	TRP B	42	26.739	-9.913	16.467
ATOM	1304	NE1	TRP B	42	27.548	-9.191	14.533
ATOM	1305	HE1	TRP B	42	28.067	-8.702	13.818
ATOM	1306	CE2	TRP B	42	27.664	-8.995	15.893
ATOM	1307	CE3	TRP B	42	26.640	-9.923	17.875
ATOM	1308	CZ2	TRP B	42	28.443	-8.136	16.680
ATOM	1309	CZ3	TRP B	42	27.426	-9.075	18.673
ATOM	1310	CH2	TRP B	42	28.318	-8.171	18.077
ATOM	1311	N	LYS B	43	23.416	-13.980	16.617
ATOM	1312	H	LYS B	43	23.105	-13.044	16.840
ATOM	1313	CA	LYS B	43	22.378	-14.995	16.526
ATOM	1314	C	LYS B	43	21.368	-14.507	15.478
ATOM	1315	O	LYS B	43	20.743	-13.472	15.706
ATOM	1316	CB	LYS B	43	21.694	-15.196	17.893
ATOM	1317	CG	LYS B	43	22.641	-15.623	19.034
ATOM	1318	CD	LYS B	43	22.409	-14.814	20.323
ATOM	1319	CE	LYS B	43	22.767	-13.327	20.182
ATOM	1320	NZ	LYS B	43	24.214	-13.113	20.015
ATOM	1321	1HZ	LYS B	43	24.400	-12.125	19.924
ATOM	1322	3HZ	LYS B	43	24.532	-13.593	19.185
ATOM	1323	2HZ	LYS B	43	24.702	-13.476	20.821
ATOM	1324	N	PRO B	44	21.175	-15.204	14.341
ATOM	1325	CA	PRO B	44	20.139	-14.835	13.382
ATOM	1326	C	PRO B	44	18.765	-14.997	14.044
ATOM	1327	O	PRO B	44	18.573	-15.902	14.860
ATOM	1328	CB	PRO B	44	20.341	-15.761	12.180
ATOM	1329	CG	PRO B	44	20.999	-16.999	12.787
ATOM	1330	CD	PRO B	44	21.837	-16.434	13.933
ATOM	1331	N	LYS B	45	17.825	-14.101	13.712
ATOM	1332	H	LYS B	45	17.994	-13.483	12.944
ATOM	1333	CA	LYS B	45	16.523	-14.088	14.339
ATOM	1334	C	LYS B	45	15.519	-13.590	13.329
ATOM	1335	O	LYS B	45	15.829	-12.838	12.379
ATOM	1336	CB	LYS B	45	16.558	-13.149	15.560
ATOM	1337	CG	LYS B	45	15.469	-13.442	16.579
ATOM	1338	CD	LYS B	45	15.256	-12.254	17.501
ATOM	1339	CE	LYS B	45	14.131	-12.461	18.469
ATOM	1340	NZ	LYS B	45	14.549	-13.442	19.474
ATOM	1341	1HZ	LYS B	45	13.805	-13.588	20.126
ATOM	1342	3HZ	LYS B	45	15.355	-13.101	19.958

FIG. 1 IX

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ATOM	1343	2HZ	LYS	B	45	14.772	-14.306	19.023
ATOM	1344	N	MET	B	46	14.240	-14.005	13.416
ATOM	1345	H	MET	B	46	13.991	-14.705	14.085
ATOM	1346	CA	MET	B	46	13.203	-13.472	12.570
ATOM	1347	C	MET	B	46	12.291	-12.623	13.425
ATOM	1348	O	MET	B	46	11.782	-13.063	14.471
ATOM	1349	CB	MET	B	46	12.383	-14.616	12.016
ATOM	1350	CG	MET	B	46	13.153	-15.586	11.187
ATOM	1351	SD	MET	B	46	12.977	-15.188	9.473
ATOM	1352	CE	MET	B	46	13.566	-16.690	8.775
ATOM	1353	N	ILE	B	47	11.933	-11.379	13.030
ATOM	1354	H	ILE	B	47	12.327	-10.991	12.196
ATOM	1355	CA	ILE	B	47	10.971	-10.568	13.797
ATOM	1356	C	ILE	B	47	9.761	-10.233	12.962
ATOM	1357	O	ILE	B	47	9.819	-10.048	11.731
ATOM	1358	CB	ILE	B	47	11.608	-9.294	14.385
ATOM	1359	CG1	ILE	B	47	12.345	-8.459	13.318
ATOM	1360	CG2	ILE	B	47	12.542	-9.638	15.494
ATOM	1361	CD1	ILE	B	47	12.789	-7.123	13.851
ATOM	1362	N	GLY	B	48	8.557	-10.136	13.558
ATOM	1363	H	GLY	B	48	8.484	-10.249	14.549
ATOM	1364	CA	GLY	B	48	7.365	-9.872	12.800
ATOM	1365	C	GLY	B	48	6.826	-8.512	13.141
ATOM	1366	O	GLY	B	48	7.136	-7.832	14.149
ATOM	1367	N	GLY	B	49	5.940	-8.027	12.306
ATOM	1368	H	GLY	B	49	5.668	-8.562	11.506
ATOM	1369	CA	GLY	B	49	5.336	-6.745	12.493
ATOM	1370	C	GLY	B	49	4.082	-6.786	11.674
ATOM	1371	O	GLY	B	49	3.561	-7.847	11.273
ATOM	1372	N	ILE	B	50	3.531	-5.634	11.315
ATOM	1373	H	ILE	B	50	4.015	-4.777	11.492
ATOM	1374	CA	ILE	B	50	2.247	-5.573	10.673
ATOM	1375	C	ILE	B	50	2.118	-6.456	9.420
ATOM	1376	O	ILE	B	50	1.175	-7.253	9.215
ATOM	1377	CB	ILE	B	50	1.982	-4.071	10.391
ATOM	1378	CG1	ILE	B	50	1.005	-3.539	11.396
ATOM	1379	CG2	ILE	B	50	1.610	-3.739	8.922
ATOM	1380	CD1	ILE	B	50	-0.391	-4.077	11.252
ATOM	1381	N	GLY	B	51	3.113	-6.410	8.519
ATOM	1382	H	GLY	B	51	3.957	-5.920	8.737
ATOM	1383	CA	GLY	B	51	2.926	-7.075	7.259
ATOM	1384	C	GLY	B	51	3.671	-8.391	7.077
ATOM	1385	O	GLY	B	51	3.716	-8.945	5.973
ATOM	1386	N	GLY	B	52	4.296	-8.982	8.116
ATOM	1387	H	GLY	B	52	4.227	-8.580	9.029
ATOM	1388	CA	GLY	B	52	5.053	-10.190	7.874
ATOM	1389	C	GLY	B	52	6.334	-10.178	8.678
ATOM	1390	O	GLY	B	52	6.519	-9.421	9.657
ATOM	1391	N	PHE	B	53	7.325	-11.015	8.343
ATOM	1392	H	PHE	B	53	7.227	-11.603	7.540
ATOM	1393	CA	PHE	B	53	8.542	-11.096	9.110
ATOM	1394	C	PHE	B	53	9.727	-10.584	8.315
ATOM	1395	O	PHE	B	53	9.780	-10.618	7.075
ATOM	1396	CB	PHE	B	53	8.804	-12.555	9.542
ATOM	1397	CG	PHE	B	53	7.850	-13.023	10.592
ATOM	1398	CD1	PHE	B	53	6.513	-13.277	10.279

FIG. 1IY

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```
ATOM   1399  CD2 PHE B  53       8.279 -13.192  11.918
ATOM   1400  CE1 PHE B  53       5.620 -13.697  11.253
ATOM   1401  CE2 PHE B  53       7.382 -13.615  12.903
ATOM   1402  CZ  PHE B  53       6.052 -13.868  12.574
ATOM   1403  N   ILE B  54      10.758 -10.126   8.985
ATOM   1404  H   ILE B  54      10.665  -9.922   9.960
ATOM   1405  CA  ILE B  54      12.029  -9.910   8.338
ATOM   1406  C   ILE B  54      13.089 -10.648   9.134
ATOM   1407  O   ILE B  54      12.952 -11.006  10.325
ATOM   1408  CB  ILE B  54      12.390  -8.444   8.236
ATOM   1409  CG1 ILE B  54      12.386  -7.775   9.611
ATOM   1410  CG2 ILE B  54      11.460  -7.770   7.218
ATOM   1411  CD1 ILE B  54      13.113  -6.438   9.590
ATOM   1412  N   LYS B  55      14.272 -10.682   8.523
ATOM   1413  H   LYS B  55      14.383 -10.599   7.562
ATOM   1414  CA  LYS B  55      15.403 -11.431   9.216
ATOM   1415  C   LYS B  55      16.274 -10.324   9.732
ATOM   1416  O   LYS B  55      16.620  -9.328   9.047
ATOM   1417  CB  LYS B  55      16.222 -12.237   8.245
ATOM   1418  CG  LYS B  55      15.638 -13.596   8.063
ATOM   1419  CD  LYS B  55      16.299 -14.348   6.953
ATOM   1420  CE  LYS B  55      15.311 -14.520   5.813
ATOM   1421  NZ  LYS B  55      15.757 -15.577   4.897
ATOM   1422 1HZ  LYS B  55      15.095 -15.676   4.154
ATOM   1423 3HZ  LYS B  55      15.830 -16.441   5.395
ATOM   1424 2HZ  LYS B  55      16.650 -15.334   4.518
ATOM   1425  N   VAL B  56      16.880 -10.547  10.910
ATOM   1426  H   VAL B  56      16.741 -11.418  11.382
ATOM   1427  CA  VAL B  56      17.732  -9.578  11.534
ATOM   1428  C   VAL B  56      18.884 -10.304  12.184
ATOM   1429  O   VAL B  56      18.884 -11.518  12.367
ATOM   1430  CB  VAL B  56      16.912  -8.819  12.609
ATOM   1431  CG1 VAL B  56      15.865  -7.943  11.921
ATOM   1432  CG2 VAL B  56      16.215  -9.788  13.599
ATOM   1433  N   ARG B  57      19.958  -9.593  12.591
ATOM   1434  H   ARG B  57      20.030  -8.624  12.353
ATOM   1435  CA  ARG B  57      21.050 -10.193  13.386
ATOM   1436  C   ARG B  57      20.963  -9.608  14.804
ATOM   1437  O   ARG B  57      20.814  -8.395  15.053
ATOM   1438  CB  ARG B  57      22.426  -9.873  12.817
ATOM   1439  CG  ARG B  57      22.664 -10.437  11.439
ATOM   1440  CD  ARG B  57      24.012 -10.065  10.899
ATOM   1441  NE  ARG B  57      24.280 -10.697   9.617
ATOM   1442  HE  ARG B  57      23.592 -11.323   9.250
ATOM   1443  CZ  ARG B  57      25.392 -10.478   8.921
ATOM   1444  NH1 ARG B  57      26.337  -9.650   9.353
ATOM   1445 2HH1 ARG B  57      26.223  -9.171  10.224
ATOM   1446 1HH1 ARG B  57      27.163  -9.505   8.808
ATOM   1447  NH2 ARG B  57      25.561 -11.104   7.760
ATOM   1448 1HH2 ARG B  57      26.392 -10.950   7.225
ATOM   1449 2HH2 ARG B  57      24.857 -11.729   7.422
ATOM   1450  N   GLN B  58      20.997 -10.489  15.832
ATOM   1451  H   GLN B  58      21.176 -11.456  15.650
ATOM   1452  CA  GLN B  58      20.780 -10.072  17.206
ATOM   1453  C   GLN B  58      22.108  -9.886  17.882
ATOM   1454  O   GLN B  58      22.918 -10.815  18.038
```

FIG. 1 IZ

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ATOM	1455	CB	GLN	B	58	20.051	-11.190	17.932
ATOM	1456	CG	GLN	B	58	19.765	-10.845	19.366
ATOM	1457	CD	GLN	B	58	19.179	-12.003	20.112
ATOM	1458	OE1	GLN	B	58	19.712	-12.472	21.101
ATOM	1459	NE2	GLN	B	58	18.055	-12.476	19.623
ATOM	1460	1HE2	GLN	B	58	17.598	-13.249	20.063
ATOM	1461	2HE2	GLN	B	58	17.647	-12.066	18.807
ATOM	1462	N	TYR	B	59	22.416	-8.692	18.422
ATOM	1463	H	TYR	B	59	21.788	-7.921	18.311
ATOM	1464	CA	TYR	B	59	23.631	-8.486	19.161
ATOM	1465	C	TYR	B	59	23.244	-8.290	20.607
ATOM	1466	O	TYR	B	59	22.178	-7.728	20.927
ATOM	1467	CB	TYR	B	59	24.387	-7.241	18.653
ATOM	1468	CG	TYR	B	59	24.271	-7.075	17.149
ATOM	1469	CD1	TYR	B	59	23.045	-7.242	16.494
ATOM	1470	CD2	TYR	B	59	25.385	-6.753	16.374
ATOM	1471	CE1	TYR	B	59	22.939	-7.093	15.112
ATOM	1472	CE2	TYR	B	59	25.291	-6.603	14.995
ATOM	1473	CZ	TYR	B	59	24.068	-6.774	14.365
ATOM	1474	OH	TYR	B	59	24.018	-6.620	13.010
ATOM	1475	HH	TYR	B	59	24.926	-6.394	12.658
ATOM	1476	N	ASP	B	60	24.010	-8.785	21.596
ATOM	1477	H	ASP	B	60	24.852	-9.276	21.372
ATOM	1478	CA	ASP	B	60	23.644	-8.624	22.992
ATOM	1479	C	ASP	B	60	24.556	-7.595	23.615
ATOM	1480	O	ASP	B	60	25.654	-7.261	23.125
ATOM	1481	CB	ASP	B	60	23.789	-9.920	23.777
ATOM	1482	CG	ASP	B	60	22.803	-10.960	23.332
ATOM	1483	OD1	ASP	B	60	21.619	-10.634	23.032
ATOM	1484	OD2	ASP	B	60	23.208	-12.126	23.273
ATOM	1485	N	GLN	B	61	24.156	-7.022	24.774
ATOM	1486	H	GLN	B	61	23.252	-7.234	25.146
ATOM	1487	CA	GLN	B	61	25.011	-6.086	25.519
ATOM	1488	C	GLN	B	61	25.411	-4.866	24.746
ATOM	1489	O	GLN	B	61	26.560	-4.382	24.832
ATOM	1490	CB	GLN	B	61	26.269	-6.763	26.028
ATOM	1491	CG	GLN	B	61	26.020	-8.038	26.753
ATOM	1492	CD	GLN	B	61	25.714	-7.766	28.185
ATOM	1493	OE1	GLN	B	61	24.572	-7.455	28.548
ATOM	1494	NE2	GLN	B	61	26.744	-7.844	29.014
ATOM	1495	1HE2	GLN	B	61	26.620	-7.675	29.992
ATOM	1496	2HE2	GLN	B	61	27.654	-8.073	28.669
ATOM	1497	N	ILE	B	62	24.539	-4.257	23.933
ATOM	1498	H	ILE	B	62	23.628	-4.648	23.801
ATOM	1499	CA	ILE	B	62	24.878	-3.047	23.238
ATOM	1500	C	ILE	B	62	24.571	-1.885	24.144
ATOM	1501	O	ILE	B	62	23.515	-1.819	24.819
ATOM	1502	CB	ILE	B	62	24.097	-2.922	21.912
ATOM	1503	CG1	ILE	B	62	24.310	-4.170	21.094
ATOM	1504	CG2	ILE	B	62	24.568	-1.709	21.067
ATOM	1505	CD1	ILE	B	62	25.794	-4.479	20.878
ATOM	1506	N	LEU	B	63	25.485	-0.912	24.304
ATOM	1507	H	LEU	B	63	26.403	-1.028	23.926
ATOM	1508	CA	LEU	B	63	25.192	0.322	25.015
ATOM	1509	C	LEU	B	63	24.630	1.296	24.030
ATOM	1510	O	LEU	B	63	25.239	1.658	22.995

FIG. I laa

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ATOM	1511	CB	LEU	B	63	26.436	0.970	25.590
ATOM	1512	CG	LEU	B	63	26.186	2.358	26.226
ATOM	1513	CD1	LEU	B	63	25.486	2.261	27.576
ATOM	1514	CD2	LEU	B	63	27.468	3.162	26.382
ATOM	1515	N	ILE	B	64	23.492	1.946	24.358
ATOM	1516	H	ILE	B	64	22.958	1.643	25.148
ATOM	1517	CA	ILE	B	64	23.003	3.068	23.617
ATOM	1518	C	ILE	B	64	22.872	4.194	24.612
ATOM	1519	O	ILE	B	64	22.915	4.007	25.846
ATOM	1520	CB	ILE	B	64	21.634	2.701	22.989
ATOM	1521	CG1	ILE	B	64	21.825	1.521	22.029
ATOM	1522	CG2	ILE	B	64	20.982	3.894	22.246
ATOM	1523	CD1	ILE	B	64	20.593	1.096	21.260
ATOM	1524	N	GLU	B	65	22.803	5.460	24.172
ATOM	1525	H	GLU	B	65	23.013	5.664	23.216
ATOM	1526	CA	GLU	B	65	22.432	6.551	25.037
ATOM	1527	C	GLU	B	65	21.242	7.194	24.373
ATOM	1528	O	GLU	B	65	21.312	7.729	23.257
ATOM	1529	CB	GLU	B	65	23.497	7.615	25.131
ATOM	1530	CG	GLU	B	65	24.787	7.196	25.761
ATOM	1531	CD	GLU	B	65	25.694	8.385	26.076
ATOM	1532	OE1	GLU	B	65	25.170	9.510	26.311
ATOM	1533	OE2	GLU	B	65	26.938	8.200	26.092
ATOM	1534	N	ILE	B	66	20.078	7.240	25.035
ATOM	1535	H	ILE	B	66	20.010	6.835	25.947
ATOM	1536	CA	ILE	B	66	18.907	7.865	24.462
ATOM	1537	C	ILE	B	66	18.777	9.195	25.145
ATOM	1538	O	ILE	B	66	18.591	9.303	26.379
ATOM	1539	CB	ILE	B	66	17.713	6.995	24.790
ATOM	1540	CG1	ILE	B	66	17.916	5.583	24.335
ATOM	1541	CG2	ILE	B	66	16.405	7.544	24.177
ATOM	1542	CD1	ILE	B	66	16.888	4.677	24.884
ATOM	1543	N	CYS	B	67	18.965	10.325	24.437
ATOM	1544	H	CYS	B	67	19.201	10.268	23.467
ATOM	1545	CA	CYS	B	67	18.833	11.663	25.049
ATOM	1546	C	CYS	B	67	19.637	11.781	26.319
ATOM	1547	O	CYS	B	67	19.235	12.400	27.328
ATOM	1548	CB	CYS	B	67	17.387	12.023	25.319
ATOM	1549	SG	CYS	B	67	16.407	12.259	23.821
ATOM	1550	N	GLY	B	68	20.830	11.180	26.383
ATOM	1551	H	GLY	B	68	21.158	10.646	25.604
ATOM	1552	CA	GLY	B	68	21.654	11.268	27.558
ATOM	1553	C	GLY	B	68	21.464	10.185	28.584
ATOM	1554	O	GLY	B	68	22.174	10.128	29.606
ATOM	1555	N	HIS	B	69	20.513	9.255	28.425
ATOM	1556	H	HIS	B	69	19.924	9.282	27.618
ATOM	1557	CA	HIS	B	69	20.304	8.199	29.391
ATOM	1558	C	HIS	B	69	20.861	6.936	28.811
ATOM	1559	O	HIS	B	69	20.589	6.560	27.647
ATOM	1560	CB	HIS	B	69	18.832	7.992	29.654
ATOM	1561	CG	HIS	B	69	18.175	9.203	30.223
ATOM	1562	ND1	HIS	B	69	17.504	9.195	31.435
ATOM	1563	HD1	HIS	B	69	17.383	8.402	32.032
ATOM	1564	CD2	HIS	B	69	18.122	10.470	29.729
ATOM	1565	CE1	HIS	B	69	17.070	10.429	31.626
ATOM	1566	NE2	HIS	B	69	17.410	11.240	30.635

FIG. 1 lbb

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ATOM	1567	N	LYS	B	70	21.751	6.217	29.499
ATOM	1568	H	LYS	B	70	22.025	6.512	30.414
ATOM	1569	CA	LYS	B	70	22.326	5.020	28.945
ATOM	1570	C	LYS	B	70	21.386	3.854	29.145
ATOM	1571	O	LYS	B	70	20.627	3.725	30.120
ATOM	1572	CB	LYS	B	70	23.613	4.678	29.663
ATOM	1573	CG	LYS	B	70	24.694	5.655	29.379
ATOM	1574	CD	LYS	B	70	25.739	5.524	30.444
ATOM	1575	CE	LYS	B	70	27.048	6.090	30.011
ATOM	1576	NZ	LYS	B	70	26.948	7.548	30.000
ATOM	1577	1HZ	LYS	B	70	27.821	7.940	29.711
ATOM	1578	3HZ	LYS	B	70	26.725	7.874	30.919
ATOM	1579	2HZ	LYS	B	70	26.230	7.828	29.363
ATOM	1580	N	ALA	B	71	21.512	2.849	28.284
ATOM	1581	H	ALA	B	71	22.141	2.934	27.512
ATOM	1582	CA	ALA	B	71	20.762	1.630	28.432
ATOM	1583	C	ALA	B	71	21.629	0.576	27.805
ATOM	1584	O	ALA	B	71	22.463	0.830	26.912
ATOM	1585	CB	ALA	B	71	19.452	1.726	27.737
ATOM	1586	N	ILE	B	72	21.547	-0.681	28.237
ATOM	1587	H	ILE	B	72	20.864	-0.925	28.926
ATOM	1588	CA	ILE	B	72	22.424	-1.698	27.730
ATOM	1589	C	ILE	B	72	21.615	-2.938	27.462
ATOM	1590	O	ILE	B	72	20.909	-3.490	28.330
ATOM	1591	CB	ILE	B	72	23.524	-1.999	28.737
ATOM	1592	CG1	ILE	B	72	24.322	-0.735	29.090
ATOM	1593	CG2	ILE	B	72	24.442	-3.037	28.153
ATOM	1594	CD1	ILE	B	72	25.374	-1.012	30.163
ATOM	1595	N	GLY	B	73	21.609	-3.446	26.235
ATOM	1596	H	GLY	B	73	22.204	-3.054	25.534
ATOM	1597	CA	GLY	B	73	20.707	-4.545	26.062
ATOM	1598	C	GLY	B	73	20.828	-5.084	24.663
ATOM	1599	O	GLY	B	73	21.754	-4.831	23.863
ATOM	1600	N	THR	B	74	19.856	-5.905	24.271
ATOM	1601	H	THR	B	74	19.086	-6.088	24.882
ATOM	1602	CA	THR	B	74	19.869	-6.548	22.988
ATOM	1603	C	THR	B	74	19.363	-5.590	21.931
ATOM	1604	O	THR	B	74	18.338	-4.870	22.053
ATOM	1605	CB	THR	B	74	19.011	-7.801	23.074
ATOM	1606	OG1	THR	B	74	19.611	-8.683	24.013
ATOM	1607	HG1	THR	B	74	19.068	-9.519	24.092
ATOM	1608	CG2	THR	B	74	18.817	-8.496	21.705
ATOM	1609	N	VAL	B	75	20.028	-5.620	20.762
ATOM	1610	H	VAL	B	75	20.835	-6.203	20.666
ATOM	1611	CA	VAL	B	75	19.630	-4.837	19.611
ATOM	1612	C	VAL	B	75	19.600	-5.771	18.426
ATOM	1613	O	VAL	B	75	20.444	-6.673	18.230
ATOM	1614	CB	VAL	B	75	20.667	-3.712	19.395
ATOM	1615	CG1	VAL	B	75	20.473	-3.002	18.046
ATOM	1616	CG2	VAL	B	75	20.679	-2.708	20.567
ATOM	1617	N	LEU	B	76	18.557	-5.647	17.565
ATOM	1618	H	LEU	B	76	17.822	-5.000	17.767
ATOM	1619	CA	LEU	B	76	18.444	-6.427	16.324
ATOM	1620	C	LEU	B	76	18.736	-5.487	15.144
ATOM	1621	O	LEU	B	76	18.239	-4.343	15.040
ATOM	1622	CB	LEU	B	76	17.028	-7.021	16.158

FIG. 1lcc

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ATOM	1623	CG	LEU	B	76	16.427	-7.612	17.449
ATOM	1624	CD1	LEU	B	76	14.992	-8.075	17.263
ATOM	1625	CD2	LEU	B	76	17.266	-8.758	18.019
ATOM	1626	N	VAL	B	77	19.607	-5.900	14.222
ATOM	1627	H	VAL	B	77	19.985	-6.824	14.276
ATOM	1628	CA	VAL	B	77	20.027	-5.042	13.133
ATOM	1629	C	VAL	B	77	19.570	-5.662	11.842
ATOM	1630	O	VAL	B	77	19.678	-6.883	11.598
ATOM	1631	CB	VAL	B	77	21.563	-4.905	13.191
ATOM	1632	CG1	VAL	B	77	22.129	-4.202	11.944
ATOM	1633	CG2	VAL	B	77	22.030	-4.166	14.470
ATOM	1634	N	GLY	B	78	18.978	-4.915	10.943
ATOM	1635	H	GLY	B	78	18.841	-3.941	11.121
ATOM	1636	CA	GLY	B	78	18.523	-5.475	9.705
ATOM	1637	C	GLY	B	78	18.019	-4.338	8.874
ATOM	1638	O	GLY	B	78	18.130	-3.142	9.223
ATOM	1639	N	PRO	B	79	17.408	-4.596	7.722
ATOM	1640	CA	PRO	B	79	16.954	-3.535	6.834
ATOM	1641	C	PRO	B	79	15.635	-2.872	7.280
ATOM	1642	O	PRO	B	79	14.609	-2.877	6.565
ATOM	1643	CB	PRO	B	79	16.804	-4.274	5.492
ATOM	1644	CG	PRO	B	79	16.463	-5.712	5.881
ATOM	1645	CD	PRO	B	79	17.159	-5.959	7.189
ATOM	1646	N	THR	B	80	15.574	-2.247	8.458
ATOM	1647	H	THR	B	80	16.374	-2.242	9.058
ATOM	1648	CA	THR	B	80	14.364	-1.583	8.865
ATOM	1649	C	THR	B	80	14.312	-0.189	8.228
ATOM	1650	O	THR	B	80	15.349	0.471	8.001
ATOM	1651	CB	THR	B	80	14.250	-1.512	10.410
ATOM	1652	OG1	THR	B	80	13.079	-0.802	10.806
ATOM	1653	HG1	THR	B	80	13.022	-0.766	11.804
ATOM	1654	CG2	THR	B	80	15.519	-0.901	11.062
ATOM	1655	N	PRO	B	81	13.137	0.354	7.885
ATOM	1656	CA	PRO	B	81	13.036	1.747	7.379
ATOM	1657	C	PRO	B	81	13.363	2.732	8.484
ATOM	1658	O	PRO	B	81	13.791	3.880	8.250
ATOM	1659	CB	PRO	B	81	11.548	1.912	6.982
ATOM	1660	CG	PRO	B	81	10.819	0.674	7.488
ATOM	1661	CD	PRO	B	81	11.854	-0.387	7.797
ATOM	1662	N	VAL	B	82	13.197	2.368	9.772
ATOM	1663	H	VAL	B	82	12.940	1.427	9.992
ATOM	1664	CA	VAL	B	82	13.380	3.306	10.885
ATOM	1665	C	VAL	B	82	14.160	2.668	12.010
ATOM	1666	O	VAL	B	82	14.045	1.465	12.293
ATOM	1667	CB	VAL	B	82	11.996	3.695	11.431
ATOM	1668	CG1	VAL	B	82	12.055	4.961	12.269
ATOM	1669	CG2	VAL	B	82	10.958	3.857	10.318
ATOM	1670	N	ASN	B	83	14.963	3.422	12.775
ATOM	1671	H	ASN	B	83	15.147	4.370	12.516
ATOM	1672	CA	ASN	B	83	15.550	2.846	13.967
ATOM	1673	C	ASN	B	83	14.481	2.874	15.022
ATOM	1674	O	ASN	B	83	13.814	3.903	15.294
ATOM	1675	CB	ASN	B	83	16.743	3.639	14.472
ATOM	1676	CG	ASN	B	83	17.935	3.574	13.570
ATOM	1677	OD1	ASN	B	83	18.409	2.511	13.167
ATOM	1678	ND2	ASN	B	83	18.439	4.735	13.238

FIG. 1 ldd

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ATOM	1679	2HD2	ASN	B	83	19.237	4.786	12.638
ATOM	1680	1HD2	ASN	B	83	18.030	5.580	13.582
ATOM	1681	N	ILE	B	84	14.225	1.749	15.711
ATOM	1682	H	ILE	B	84	14.791	0.938	15.564
ATOM	1683	CA	ILE	B	84	13.154	1.658	16.667
ATOM	1684	C	ILE	B	84	13.740	1.317	18.020
ATOM	1685	O	ILE	B	84	14.428	0.300	18.223
ATOM	1686	CB	ILE	B	84	12.214	0.517	16.260
ATOM	1687	CG1	ILE	B	84	11.656	0.759	14.849
ATOM	1688	CG2	ILE	B	84	11.128	0.247	17.315
ATOM	1689	CD1	ILE	B	84	10.770	-0.359	14.291
ATOM	1690	N	ILE	B	85	13.483	2.157	19.051
ATOM	1691	H	ILE	B	85	13.028	3.030	18.877
ATOM	1692	CA	ILE	B	85	13.846	1.834	20.408
ATOM	1693	C	ILE	B	85	12.596	1.254	21.085
ATOM	1694	O	ILE	B	85	11.536	1.903	21.267
ATOM	1695	CB	ILE	B	85	14.308	3.115	21.137
ATOM	1696	CG1	ILE	B	85	15.447	3.826	20.395
ATOM	1697	CG2	ILE	B	85	14.673	2.840	22.589
ATOM	1698	CD1	ILE	B	85	16.730	3.053	20.263
ATOM	1699	N	GLY	B	86	12.617	-0.052	21.422
ATOM	1700	H	GLY	B	86	13.439	-0.595	21.251
ATOM	1701	CA	GLY	B	86	11.481	-0.702	22.028
ATOM	1702	C	GLY	B	86	11.557	-0.748	23.538
ATOM	1703	O	GLY	B	86	12.412	-0.165	24.238
ATOM	1704	N	ARG	B	87	10.614	-1.489	24.149
ATOM	1705	H	ARG	B	87	10.012	-2.072	23.604
ATOM	1706	CA	ARG	B	87	10.442	-1.468	25.584
ATOM	1707	C	ARG	B	87	11.627	-2.021	26.326
ATOM	1708	O	ARG	B	87	11.911	-1.666	27.495
ATOM	1709	CB	ARG	B	87	9.200	-2.271	25.949
ATOM	1710	CG	ARG	B	87	7.951	-1.960	25.161
ATOM	1711	CD	ARG	B	87	6.956	-3.074	25.219
ATOM	1712	NE	ARG	B	87	5.906	-2.933	24.205
ATOM	1713	HE	ARG	B	87	5.790	-2.039	23.772
ATOM	1714	CZ	ARG	B	87	5.119	-3.953	23.856
ATOM	1715	NH1	ARG	B	87	5.252	-5.161	24.396
ATOM	1716	2HH1	ARG	B	87	5.958	-5.326	25.085
ATOM	1717	1HH1	ARG	B	87	4.646	-5.905	24.113
ATOM	1718	NH2	ARG	B	87	4.180	-3.751	22.939
ATOM	1719	1HH2	ARG	B	87	3.580	-4.502	22.664
ATOM	1720	2HH2	ARG	B	87	4.073	-2.848	22.524
ATOM	1721	N	ASN	B	88	12.413	-2.937	25.731
ATOM	1722	H	ASN	B	88	12.206	-3.237	24.800
ATOM	1723	CA	ASN	B	88	13.582	-3.519	26.415
ATOM	1724	C	ASN	B	88	14.532	-2.429	26.821
ATOM	1725	O	ASN	B	88	15.214	-2.516	27.863
ATOM	1726	CB	ASN	B	88	14.285	-4.605	25.559
ATOM	1727	CG	ASN	B	88	15.063	-4.031	24.358
ATOM	1728	OD1	ASN	B	88	14.515	-3.245	23.612
ATOM	1729	ND2	ASN	B	88	16.333	-4.445	24.180
ATOM	1730	2HD2	ASN	B	88	16.875	-4.099	23.414
ATOM	1731	1HD2	ASN	B	88	16.744	-5.102	24.812
ATOM	1732	N	LEU	B	89	14.695	-1.328	26.061
ATOM	1733	H	LEU	B	89	14.192	-1.240	25.201
ATOM	1734	CA	LEU	B	89	15.597	-0.234	26.452

FIG. 1 lee

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ATOM	1735	C	LEU	B	89	14.797	0.937	27.053
ATOM	1736	O	LEU	B	89	15.293	1.734	27.879
ATOM	1737	CB	LEU	B	89	16.421	0.232	25.236
ATOM	1738	CG	LEU	B	89	17.400	-0.754	24.567
ATOM	1739	CD1	LEU	B	89	18.215	0.002	23.573
ATOM	1740	CD2	LEU	B	89	18.352	-1.458	25.570
ATOM	1741	N	LEU	B	90	13.511	1.114	26.705
ATOM	1742	H	LEU	B	90	13.082	0.486	26.056
ATOM	1743	CA	LEU	B	90	12.698	2.221	27.257
ATOM	1744	C	LEU	B	90	12.537	2.060	28.751
ATOM	1745	O	LEU	B	90	12.575	3.033	29.533
ATOM	1746	CB	LEU	B	90	11.311	2.258	26.628
ATOM	1747	CG	LEU	B	90	11.232	2.730	25.168
ATOM	1748	CD1	LEU	B	90	9.808	2.744	24.642
ATOM	1749	CD2	LEU	B	90	11.831	4.105	24.982
ATOM	1750	N	THR	B	91	12.315	0.843	29.271
ATOM	1751	H	THR	B	91	12.218	0.055	28.663
ATOM	1752	CA	THR	B	91	12.210	0.634	30.699
ATOM	1753	C	THR	B	91	13.537	1.028	31.375
ATOM	1754	O	THR	B	91	13.575	1.525	32.518
ATOM	1755	CB	THR	B	91	11.893	-0.843	31.028
ATOM	1756	OG1	THR	B	91	12.919	-1.676	30.504
ATOM	1757	HG1	THR	B	91	12.722	-2.634	30.713
ATOM	1758	CG2	THR	B	91	10.599	-1.285	30.418
ATOM	1759	N	GLN	B	92	14.705	0.852	30.732
ATOM	1760	H	GLN	B	92	14.707	0.497	29.797
ATOM	1761	CA	GLN	B	92	15.920	1.190	31.433
ATOM	1762	C	GLN	B	92	16.088	2.660	31.633
ATOM	1763	O	GLN	B	92	16.807	3.137	32.527
ATOM	1764	CB	GLN	B	92	17.127	0.680	30.682
ATOM	1765	CG	GLN	B	92	17.076	-0.805	30.517
ATOM	1766	CD	GLN	B	92	18.336	-1.314	29.900
ATOM	1767	OE1	GLN	B	92	19.394	-0.720	30.059
ATOM	1768	NE2	GLN	B	92	18.221	-2.411	29.195
ATOM	1769	1HE2	GLN	B	92	19.022	-2.813	28.751
ATOM	1770	2HE2	GLN	B	92	17.331	-2.856	29.095
ATOM	1771	N	ILE	B	93	15.538	3.512	30.746
ATOM	1772	H	ILE	B	93	15.016	3.153	29.972
ATOM	1773	CA	ILE	B	93	15.693	4.937	30.899
ATOM	1774	C	ILE	B	93	14.522	5.549	31.698
ATOM	1775	O	ILE	B	93	14.438	6.773	31.940
ATOM	1776	CB	ILE	B	93	15.981	5.657	29.548
ATOM	1777	CG1	ILE	B	93	14.746	5.718	28.619
ATOM	1778	CG2	ILE	B	93	17.223	5.060	28.874
ATOM	1779	CD1	ILE	B	93	14.946	6.734	27.488
ATOM	1780	N	GLY	B	94	13.617	4.731	32.263
ATOM	1781	H	GLY	B	94	13.639	3.752	32.060
ATOM	1782	CA	GLY	B	94	12.594	5.224	33.170
ATOM	1783	C	GLY	B	94	11.443	5.846	32.432
ATOM	1784	O	GLY	B	94	10.766	6.803	32.878
ATOM	1785	N	CYS	B	95	11.134	5.354	31.225
ATOM	1786	H	CYS	B	95	11.603	4.538	30.888
ATOM	1787	CA	CYS	B	95	10.134	5.969	30.381
ATOM	1788	C	CYS	B	95	8.750	5.512	30.764
ATOM	1789	O	CYS	B	95	8.478	4.309	31.006
ATOM	1790	CB	CYS	B	95	10.456	5.643	28.922

FIG. 1 lff

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ATOM   1791  SG   CYS B  95      9.426    6.512   27.764
ATOM   1792  N    THR B  96      7.778    6.444   30.764
ATOM   1793  H    THR B  96      8.014    7.401   30.539
ATOM   1794  CA   THR B  96      6.379    6.163   31.108
ATOM   1795  C    THR B  96      5.390    6.970   30.254
ATOM   1796  O    THR B  96      5.567    8.171   30.066
ATOM   1797  CB   THR B  96      6.111    6.439   32.604
ATOM   1798  OG1  THR B  96      6.341    7.794   32.938
ATOM   1799  HG1  THR B  96      6.111    7.924   33.861
ATOM   1800  CG2  THR B  96      6.938    5.566   33.554
ATOM   1801  N    LEU B  97      4.302    6.321   29.809
ATOM   1802  H    LEU B  97      4.216    5.332   29.997
ATOM   1803  CA   LEU B  97      3.127    6.986   29.238
ATOM   1804  C    LEU B  97      2.336    7.681   30.358
ATOM   1805  O    LEU B  97      2.350    7.221   31.499
ATOM   1806  CB   LEU B  97      2.226    5.958   28.532
ATOM   1807  CG   LEU B  97      2.860    5.279   27.300
ATOM   1808  CD1  LEU B  97      2.101    3.986   26.957
ATOM   1809  CD2  LEU B  97      2.842    6.216   26.085
ATOM   1810  N    ASN B  98      1.637    8.777   30.024
ATOM   1811  H    ASN B  98      1.662    9.086   29.063
ATOM   1812  CA   ASN B  98      0.906    9.631   30.960
ATOM   1813  C    ASN B  98     -0.251   10.321   30.231
ATOM   1814  O    ASN B  98     -0.032   11.303   29.522
ATOM   1815  CB   ASN B  98      1.845   10.678   31.587
ATOM   1816  CG   ASN B  98      2.783   10.077   32.634
ATOM   1817  OD1  ASN B  98      3.926    9.739   32.335
ATOM   1818  ND2  ASN B  98      2.297    9.942   33.870
ATOM   1819 2HD2  ASN B  98      2.877    9.551   34.599
ATOM   1820 1HD2  ASN B  98      1.351   10.229   34.074
ATOM   1821  N    LEU B  99     -1.476    9.808   30.426
ATOM   1822  H    LEU B  99     -1.568    9.010   31.037
ATOM   1823  CA   LEU B  99     -2.709   10.288   29.797
ATOM   1824  C    LEU B  99     -3.816   10.589   30.815
ATOM   1825  O    LEU B  99     -3.630   10.272   32.011
ATOM   1826  CB   LEU B  99     -3.146    9.340   28.657
ATOM   1827  CG   LEU B  99     -3.714    7.932   28.941
ATOM   1828  CD1  LEU B  99     -2.767    7.057   29.774
ATOM   1829  CD2  LEU B  99     -5.134    7.943   29.528
ATOM   1830  OXT  LEU B  99     -4.842   11.156   30.376
TER
```

FIG. 1 Igg

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Database filename: hivpr.mdb
Number of structures: 10591
Tolerance (%) >= 1.05

ResNum	TotOcc	TotFreq	Dist	WtAA	NumMut	MutList	NumList
1	11	0	15.4	P	0		
2	32	0	14.5	Q	0		
3	38	0	12.1	I	0		
4	106	0	13.0	T	0		
5	100	0	11.3	L	0		
6	47	0	14.3	W	0		
7	58	0	12.8	Q	0		
8	27	0	9.6	R	0		
9	11	0	7.9	P	0		
10	4004	37.8	9.2	L	3	IVF	3162 441 278
11	82	0	10.9	V	0		
12	1117	10.5	13.7	T	5	SEPAN	241 185 158 155 117
13	1745	16.5	13.7	I	1	V	1717
14	646	6.1	17.0	K	1	R	623
15	1760	16.6	17.5	I	1	V	1709
16	361	3.4	20.9	G	1	E	254
17	56	0	22.4	G	0		
18	242	2.3	20.5	Q	0		
19	1340	12.7	18.3	L	4	IVQT	873 162 130 128
20	1549	14.6	15.4	K	4	IRTM	576 560 209 145
21	43	0	12.7	E	0		
22	46	0	9.0	A	0		
23	89	0	5.8	L	0		
24	402	3.8	3.8	L	1	I	377

FIG. 8A

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25	28	0	0.0	D	0		
26	14	0	3.8	T	0		
27	9	0	5.5	G	0		
28	16	0	5.8	A	0		
29	34	0	8.7	D	0		
30	770	7.3	9.2	D	1	N	725
31	15	0	8.9	T	0		
32	238	2.2	10.5	V	1	I	221
33	578	5.5	12.4	L	3	VIF	207 189 172
34	88	0	15.1	E	0		
35	2790	26.3	18.6	E	1	D	2646
36	2780	26.2	20.2	M	2	IV	2549 129
37	3252	30.7	22.8	N	4	DSET	1253 1129 246 209
38	54	0	22.0	L	0		
39	302	2.9	24.9	P	1	S	133
40	19	0	25.5	G	0		
41	2249	21.2	26.0	R	1	K	2235
42	21	0	23.5	W	0		
43	372	3.5	23.7	K	2	TR	166 144
44	12	0	22.6	P	0		
45	208	2	20.0	K	1	R	170
46	2165	20.4	18.8	M	2	IL	1580 560
47	47	0	15.4	I	0		
48	445	4.2	14.9	G	1	V	385
49	17	0	12.9	G	0		
50	31	0	14.5	I	0		
51	24	0	17.6	G	0		
52	12	0	18.3	G	0		
53	408	3.9	18.1	F	1	L	360

FIG. 8B

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54	1661	15.7	18.0	I	1	V	1460
55	164	1.5	19.7	K	1	R	149
56	13	0	18.1	V	0		
57	1194	11.3	19.7	R	1	K	1162
58	341	3.2	18.6	Q	1	E	317
59	20	0	19.4	Y	0		
60	992	9.4	19.6	D	1	E	938
61	468	4.4	19.9	Q	1	E	285
62	2711	25.6	18.6	I	1	V	2685
63	8864	83.7	18.5	L	6	PASTQH	7245 380 321 266 226 162
64	2238	21.1	15.8	I	2	VL	1931 223
65	222	2.1	15.6	E	1	D	206
66	194	1.8	12.8	I	0		
67	309	2.9	14.6	C	1	S	143
68	51	0	17.5	G	0		
69	773	7.3	16.1	H	2	QY	376 206
70	478	4.5	17.0	K	1	R	359
71	3664	34.6	15.3	A	3	VTI	2301 1145 190
72	1494	14.1	17.2	I	3	VTL	650 409 126
73	1246	11.8	15.8	G	2	ST	932 185
74	658	6.2	15.4	T	2	SA	433 126
75	73	0	14.1	V	0		
76	59	0	14.6	L	0		
77	3533	33.4	16.1	V	1	I	3513
78	8	0	16.9	G	0		
79	95	0	17.2	P	0		
80	6	0	13.6	T	0		
81	7	0	13.7	P	0		
82	2208	20.8	11.0	V	2	AT	1668 284

FIG. 8C

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83	44	0	9.7	N	0		
84	1091	10.3	6.3	I	1	V	1073
85	213	2	5.7	I	1	V	198
86	16	0	5.3	G	0		
87	32	0	7.3	R	0		
88	706	6.7	10.4	N	2	DS	543 128
89	240	2.3	10.1	L	1	M	143
90	3429	32.4	8.3	L	1	M	3397
91	28	0	11.4	T	0		
92	227	2.1	13.6	Q	1	K	169
93	3095	29.5	13.1	I	1	L	3041
94	15	0	13.6	G	0		
95	100	0	10.6	C	0		
96	6	0	11.2	T	0		
97	83	0	10.7	L	0		
98	44	0	14.2	N	0		
99	35	0	16.4	F	0		

FIG. 8D

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Title: Use of Computationally Derived Protein Structures of Genetic Polymorphisms in
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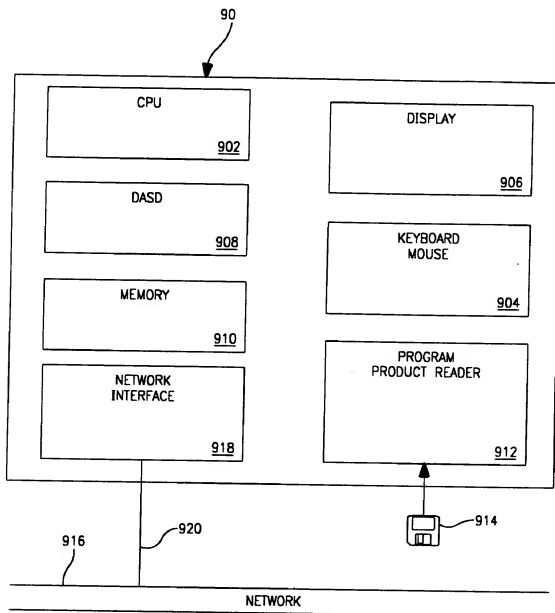Date of Filing: 11/10/00   Attorney Docket No. 24737-1906C

90

CPU

902

DISPLAY

906

DASD

908

KEYBOARD
MOUSE

904

MEMORY

910

NETWORK
INTERFACE

918

PROGRAM
PRODUCT READER

912

916

920

914

NETWORK

FIG. 9

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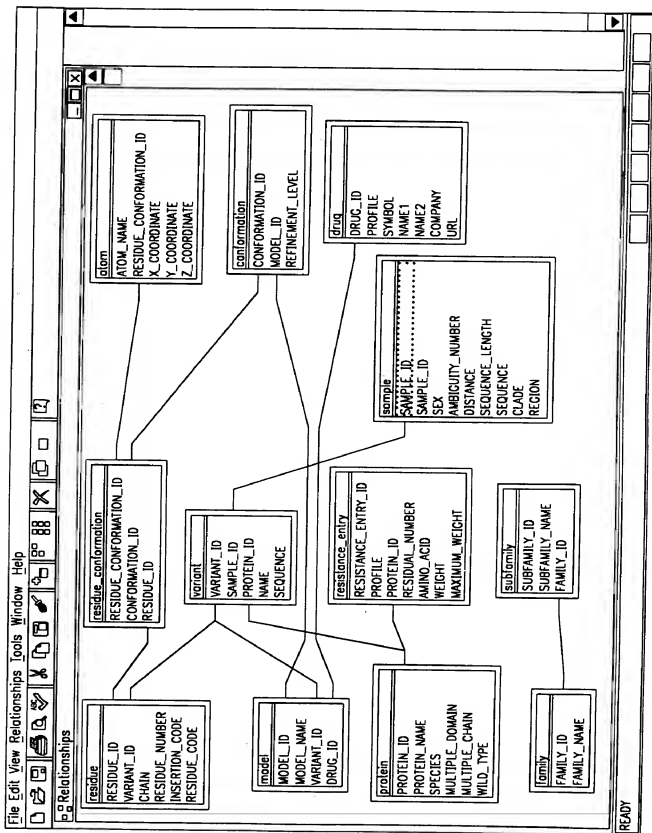Date of Filing: 11/10/00   Attorney Docket No. 24737-1906C

FIG. 10